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The Configurations $3d^n4p+3d^{n-1}4s4p+3d^{n-2}4s^24p$ in the First Spectra of the Iron Group

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Energy levels and Lande g-factors for the configurations $3d^n4p+3d^{n-1}4s4p+3d^{n-2}4s^24p$ in the first spectra of the iron group were calculated and compared with experimental values, in both general and individual treatments. The calculations were done in intermediate coupling taking into account explicity the interactions between configurations, as well as complete effective interactions of the core, and effective interactions $d-p$. Due to a successful starting point based on Hartree-Fock calculations for the Slater parameters, as well as the insertion of the effective interactions, considerable improvement was obtained compared to previous results.

On fitting 1537 levels using 67 free interaction parameters a mean error of 182 cm^{-1} was obtained. Altogether 3652 energy levels were calculated including all the levels for the configurations $3d^{n-2}4s^24p$ across the sequence. It was shown that all interaction parameters could be expressed either as linear functions, or linear functions with small quadratic corrections, of the atomic number. There was general qualitative agreement between the values of the parameters calculated using the semi-empirical method and those calculated using Hartree-Fock methods. There remained some isolated terms with large deviations. These are attributed to be due to the interactions with the configurations $(3d+4s)^n5p$, that were not considered explicitly in this analysis.

Tables comparing the experimental and calculated energy levels and Lande g-factors, as well as detailed analyses for each spectrum are given in another paper.

Key words: Iron group elements; least squares optimization; theoretical spectroscopy.

1. Introduction.

Traditionally, theoretical spectroscopists consider the radial Slater integrals as unknown parameters, obtaining their values empirically by fitting the experimental data to the calculated energy levels, and then performing least-squares optimization calculations.

For the even configurations $3d^n+3d^{n-1}4s$, and the odd configurations $3d^n4p$ in the second and third spectra of the iron group, the results were excellent, [1-4].[1] Furthermore, it was shown that the radial parameters are either linear functions, or linear functions with small quadratic corrections, of the atomic number. For the odd configurations in neutral atoms, the interactions between configurations are very strong. Thus the algebraic matrices of the configurations $(d+s)^np$ were calculated and checked by the author, [5-9]. Theoretical investigations were then performed for the configurations $(3d+4s)^n4p$ in neutral atoms of calcium, scandium, titanium, vanadium, chromium, manganese, iron, cobalt and nickel, [10-16].

Although the results were good (average r.m.s. error of 210cm^{-1}); a very disturbing feature of the results was the fact that the behavior of the final values of the radial parameters was generally far from linear.

It would be highly anomalous to have the radial parameters behave so irregularly in the first spectra. Thus, in order to overcome this discrepancy it was essential to have improved *initial* values of the radial parameters. Hence the radial parameters were first calculated using the Hartree-Fock method. Least-squares optimization calculations were then performed on these parameters *forcing* them to behave linearly, with possibly at most small quadratic corrections, as functions of the atomic number. The values thus computed were then compared with those obtained previously in individual treatments by the author, [10-16]. Whenever the Hartree-Fock values were *uniformly* higher or lower than those of the previous results, [10-16], appropriate scaling factors were utilized on the linearized Hartree-Fock values, and the latter were than used as initial parameters for this investigation.

[1]Figures in brackets indicate literature references at the end of this paper.

In this project were included the electrostatic and spin-orbit interactions of the individual configurations $3d^n4p$, $3d^{n-1}4s4p$ and $3d^{n-2}4s^24p$; the explicit electrostatic interactions between configurations $3d^n4p-3d^{n-1}4s4\,p$, $3d^{n-1}4s4p-3d^{n-2}4s^24p$ and $3d^n4p-3d^{n-2}4s^24p$; and the complete two-and three-body effective interactions of the core d electrons, as well as two-body mixed effective interactions between the $3d$ and $4p$ electrons.

The initial values of the radial parameters were then used to multiply the algebraic matrices on tape and the resulting matrices were diagonalized. Besides the eigenvalues, the diagonalization routine also yields the derivatives of the eigenvalues with respect to the parameters, the squares of the eigenvectors (percentage compositions) and the calculated Lande g values. The appropriate experimental levels were then fitted to the eigenvalues, and using the derivatives obtained in the diagonalization, least squares optimization calculations were performed. In these calculations, the improved values of the theoretical energy levels, the corrected values of the parameters including their statistical deviations and the sum of the squares of the differences between the observed and the calculated levels, were obtained. The rms error is then defined as

$$\Delta = \sqrt{\frac{\sum_{i=1}^{n} \Delta_i^2}{n-m}}$$

where the Δ_i are the differences between the observed and calculated levels, n is the number of known levels and m is the number of free parameters. The mean error is quite different from the mean deviation

$$\delta = \sqrt{\frac{\sum_{i=1}^{n} \Delta_i^2}{n}}$$

as the former takes into account the statistical effect of the number of free parameters. Hence in order for a new parameter to have physical significance, it should cause an essential decrease in the rms error, and not simply a decrease in the mean deviation.

The value of Δ is also given by the least-squares routine. The same derivatives can be used for several variations in the least squares, either imposing different conditions on the parameters, inserting the experimental levels with different assignments, or even rejecting some levels from consideration. The parameters of that variation which yielded the best results were used to perform new diagonalizations. This iterative process was continued until mathematical convergence was attained. In the present project four complete iterations were required.

The use of the same assumptions and the same approximations in all the spectra made it possible to obtain a consistent set of interaction parameters and compare the results obtained from the spectra of different elements. Due to a successful choice of the initial values of the radial parameters, it was shown that the final values can *indeed* be expressed as simple functions of the atomic number. A consistent use of such interpolation formulas for all parameters, combined eleven problems, formerly independent, into one problem. This result, which is significant by itself, very much improved the reliability of the results for those spectra where the experimental data is still scarce, and which are thus most in need of reliable predictions of the unknown levels.

This is particularly true for the configurations $3d^{n-2}4s^24p$. For each individual element there in not a sufficient number of experimental levels in order to predict even approximately the remaining levels. However, by considering a general treatment ALL the levels of the configurations $3d^{n-2}4s^24p$ for the entire sequence were calculated.

For completeness and comparison, individual least squares (ILS) were also performed for each element.

The procedures followed, a description of the various interactions considered, and an analysis of the results and significance of the different parameters are contained in this work. The tables comparing the experimental and calculated energy levels, values for all the theoretical levels specifying their percentage compositions, as well as detailed analyses for each spectrum are given in another paper, [17].

2. Effective electrostatic interactions

For the odd configurations in the first spectra of the iron group, both strong and weak configuration interactions are significant. The former arise when the perturbing and perturbed configurations are energetically close to each other and there is strong coupling of the configurations by the Coulomb field. These were taken into account by *explicitly* considering the configurations $3d^n4p$, $3d^{n-1}4s4p$, $3d^{n-2}4s^24p$ and the electrostatic interactions between them. Weak interactions occur when the perturbing configurations are well separated from the perturbed configuration, and the coupling of the Coulomb field is weak.

The individual weak interactions may not be significant, but their cumulative influence may be quite large, due to the increasing density of states as the continuum is approached. As it would be completely futile to consider each of these effects individually, the aim should be to modify the energy matrices of the principal configurations so that the major part of *all* the weakly perturbing configurations be included.

By first order perturbation theory, different configurations do not interact. In second order only those configurations interact that differ in the quantum numbers of at most two electrons. Bacher and Goudsmit, [18], have shown that the terms of the configuration l^n may be expressed as linear combinations of the terms of l^2, so that the perturbation of l^n by *all* the configurations differing from it by the state of two electrons, and being distant from it, can be accounted for by suitably modifying the terms of l^2. Hence these perturbations can be described by two-body effective interactions.

The first correction of this kind for the configurations d^n was the $\alpha L(L+1)$ correction introduced by Trees, [19-20], in the configurations $3d^54s$ of MnII and FeIII. Trees introduced his correction empirically, but Racah, [21], showed that the above effects can be described by a model or effective interaction of the form

$$2\alpha(l_1 \cdot l_2) + \beta q_{12}$$

where q_{12} is the seniority operator, [22]. For the configuration d^n this becomes

$$\alpha[L(L+1)-6n] + \beta Q$$

where

$$\begin{aligned} Q(n,v) &= \tfrac{1}{4}(n-v)(4l+4-n-v) \\ &= \tfrac{1}{4}(n-v)(12-n-v) \end{aligned} \qquad (1)$$

is the total seniority operator. Here n is the number of d electrons in the configurations d^np, v is the seniority of the d^n core term, and l is 2 as we are dealing with d electrons. The constant $-6n\alpha$ is usually incorporated into the height of the configuration. Racah, [21], showed that the $\alpha L(L+1)$ and the βQ corrections form a complete set of two-body effective interactions for the d^n configurations. This is due to the fact that together with the Slater integrals $F_0(d^2)$, $F_2(d^2)$ and $F_4(d^2)$, they form a set of five independent parameters that can represent the five terms of d^2.

Bacher and Goudsmit, [18], also showed that if the far-lying perturbing configuration differs from l^n by the state of only one electron, its effect can be described by expressing the terms of l^n as linear combinations of l^2, and modifying the values of these terms. Hence in the linear theory, the Hamiltonian in this case must be augmented by additional three-body interactions.

Rajnak and Wybourne, [23], obtained explicit formulas for the effective interactions representing the perturbation of an l^n configuration by far-lying configurations differing from it by one or two electrons or holes. Racah and Stein, [24], subsequently, developed an elegant method that considerably simplified the calculations of Rajnak and Wybourne.

If A and B represent the perturbed and perturbing configurations, respectively, and if G is the operator representing the Coulomb energy of repulsion between the electrons, $\sum_{i<j} \frac{e^2}{r_{ij}}$, then the matrix elements of the second-order perturbation produced by B on A are given approximately by

$$(A\psi|W_2|A\psi') = -\frac{1}{\Delta E}\sum_{\psi''}(A\psi|G|B\psi'')(B\psi''|G|A\psi'), \tag{2}$$

where ΔE is the distance between the centers of gravity of the two configurations, which are assumed to be well separated. According to Racah and Stein, [24], the operator G in the first factor is replaced by a "curtailed" operator g, whose matrix elements $(A'\psi|g|B'\psi'')$ are equal to those of G if $A' = A$ and $B' = B$, and vanish otherwise. Similarly, the operator G in the second factor is replaced by $\tilde{g}$, defined analogously to g. Then

$$(A\psi|W_2|A\psi') = -\frac{1}{\Delta E}\sum_{B'\psi''}(A\psi|g|B'\psi'')(B'\psi''|\tilde{g}|A\psi'), \tag{3}$$

where the summation is over the complete set $B'\psi''$. Thus,

$$(A\psi|W_2|A\psi') = -\frac{1}{\Delta E}(A\psi|\tilde{g}g|A\psi'), \tag{4}$$

and hence the electrostatic interaction between the configuration A and all the other distant configurations may be simply expressed as an effective interaction within the configuration A given by

$$W_2 = -\frac{\tilde{g}g}{\Delta E} \tag{5}$$

Then using either the above method or that of Rajnak and Wybourne, [23], we obtain that the correction term W_2, that must be added to the Hamiltonian of ℓ^n caused by the perturbation of ℓ^n by $\ell^{n-1}\ \ell'$configurations is given by

$$W_2 = -\sum_{kk'} P(kk';\ \ell\ell,\ \ell\ell')\ \phi\ (kk';\ \ell\ell,\ \ell\ell') \tag{6}$$

where

$$P(kk';\ \ell_a\ell_b,\ \ell_c\ell_d) = X(k;\ \ell_a\ell_b,\ \ell_c\ell_d) \cdot X(k';\ \ell_a\ell_b,\ell_c\ell_d)/\Delta E, \tag{7}$$

and

$$X(k;\ \ell_a\ell_b,\ \ell_c\ell_d) = (\ell_a\|C^{(k)}\|\ell_c)\,(\ell_b\|C^{(k)}\|\ell_d)R^k(\ell_a\ell_b,\ \ell_c\ell_d), \tag{8}$$

ΔE is the distance between the perturbing configuration and ℓ^n,

$$\phi\ (kk',\ \ell\ell,\ \ell\ell') = -\sum_{k''}(2k''+1)\begin{Bmatrix} k & k' & k'' \\ \ell & \ell & \ell' \end{Bmatrix}[U^{(k)}\times U^{(k'')}\times U^{(k')}]^{(0)}\ldots\ldots$$

$$+\ [\delta_{n\ell}/(2\ell+1)]\,[(U^{(k)}\cdot U^{(k)}) + (U^{(k')}\cdot U^{(k')}) - n/(2\ell+1)]\,. \tag{9}$$

For the perturbation W_2' of ℓ^n by $\ell'^{\,(4\ell'+1)}\ell^{n+1}$ we similarly obtain

$$W_2' = -\sum_{kk'} P(kk';\ \ell\ell,\ \ell\ell')\ \phi'\ (kk';\ \ell\ell,\ \ell\ell'), \tag{10}$$

where

$$\phi'\ (kk';\ \ell\ell,\ \ell\ell') = -\sum_{k''}(-1)^{(k''+1)}(2k''+1)\begin{Bmatrix} k & k' & k'' \\ \ell & \ell & \ell' \end{Bmatrix}\cdot$$

$$[U^{(k)}\times U^{(k'')}\times U^{(k')}]^{(0)} - [2\delta_{kk'}/(2k+1)]\,(U^{(k)}\cdot U^{(k)}). \tag{11}$$

The P are radial parameters; the ϕ and ϕ' are their coefficient operators.
The matrix elements of ℓ_n can be calculated by Racah algebra. The variables k and k' are even and nonzero integers that must satisfy the usual triangular conditions of the 6-j symbols. The variables k'' can assume all integral values consistent with the triangular conditions for the 6-j symbols.

The parameter T represents the perturbation of the configuration $3d^n$ by the configuration $3s3d^{n+1}$. It was first considered by Trees, [25], when he investigated the configuration $3s^23p^63d^6$, and took into account its

interaction with the configuration $3s3p^6 3d^7$. Shadmi, [26] extended the work of Trees to all configurations $3d^n + 3d^{n-1}4s + 3d^{n-2}4s^2$ in the sequence of the second spectra of the iron group by introducing a three-body effective interaction between $3d$ electrons which represented the perturbation of a configuration of the type $3s^2 3d^n$ by the configuration $3s3d^{n+1}$. Roth [3–4] included the parameters α, β and T in the configurations $3d^n 4p$ in the second and third spectra of the iron group, as well as for the configurations $3d^3 4p + 3d^2 4s4p$ in V II, [27].

Further important investigations were carried out by Shadmi, Stein, Oreg, Caspi, Goldschmidt and Starkand [28–30].

Now from (10) with $k = k' = 2$ here, we have $W_2' = -P(22;3d3d,3d3s)\phi'(22;dd,ds)$.

$$P(22\ ;\ 3\mathrm{d}3\mathrm{d},3\mathrm{d}3\mathrm{s}) = \frac{X(2\ ;\ 22,20)^2\,[R^2(dd,ds)]^2}{\Delta E}$$

$$= \frac{(2\|C^{(2)}\|2)^2(2\|C^{(2)}\|0)^2[R^2(dd,ds)]^2}{\Delta E}$$

$$= \frac{10}{7}\frac{[R^2(dd,ds)]^2}{\Delta E}\ .\ \text{Thus,}$$

$$W_2' = -\frac{10}{7}\frac{[R^2(dd,ds)]^2}{\Delta E}\,\phi'(22\ ;\ dd,ds)$$

$$= -\frac{10}{7}\frac{(35)^2H^2}{\Delta E}\,\phi'(22\ ;\ dd,ds)$$

$$= -\ 1750\,\frac{H^2}{\Delta E}\,\phi'(22;\ dd,ds),$$

where we used $H = \dfrac{R^2(dd,ds)}{35}$ according to Racah, [22]. However, in order to be consistant with the definition of

$$T = \frac{H^2}{\Delta E}$$

used in a previous work by the author, [7], we get for the coefficient operator of T the expression

$$t = -\ 1750\,\phi'(22;\ dd,ds). \tag{12}$$

The parameters T_x, T_y, T_z represent the perturbation of the configuration $3d^n$ by a configuration of the type $3d^{n-1}n'd$, where $n' \geqslant 4$. Similarly, to the above result for t their coefficient operators t_x, t_y, t_z are

$$t_x = -\ 1750\,\phi(22;\ dd,dd'), \tag{13a}$$
$$t_y = -\ 1750\,[\phi(24;\ dd,dd') + \phi(42;\ dd,dd')], \tag{13b}$$
$$t_z = -\ 1750\,\phi(44;\ dd,dd'). \tag{13c}$$

In terms of the P, the parameters are given by

$$T = (1/1750)P(22;\ 3d3d,\ 3d3s), \tag{14a}$$
$$T_x = (1/1750)P(22;\ 3d3d,\ 3dn'd), \tag{14b}$$
$$T_y = (1/1750)P(24;\ 3d3d,\ 3dn'd), \tag{14c}$$
$$T_z = (1/1750)P(44;\ 3d3d,\ 3dn'd). \tag{14d}$$

Only the parameters T and T_x were used as T_y and T_z depend upon the other parameters.

2.1. Effective interactions in the configuration $\ell^n\ell'$

First we define the tensor operators $u^{(k)}$, $v^{(k)}$, $w^{(k)}$, $\tilde{w}^{(k)}$, $y^{(k)}$, $\tilde{y}^{(k)}$, $z^{(k)}$ and $\tilde{z}^{(k)}$ as the tensor operators of order k whose only non-vanishing reduced matrix elements are

$$(n\ell\|u^{(k)}\|n\ell) = 1, \tag{15a}$$
$$(n'\ell'\|v^{(k)}\|n'\ell') = 1, \tag{15b}$$
$$(n'\ell'\|w^{(k)}\|n''\ell'') = (n''\ell''\|\tilde{w}^{(k)}\|n'\ell') = 1, \tag{15c}$$
$$(n\ell\|y^{(k)}\|n''\ell'') = (n''\ell''\|\tilde{y}^{(k)}\|n\ell) = 1, \tag{15d}$$
$$(n\ell\|z^{(k)}\|n'\ell') = (n'\ell'\|\tilde{z}^{(k)}\|n\ell) = 1. \tag{15e}$$

Then in terms of the quantities P and X defined in (7) and (8), the curtailed operators g and $\tilde{g}$ representing the effective interactions of the configuration $\ell^n\ell'$, may be written as

$$g = \sum_k [X(k;\ell\ell',\ell\ell'')\sum_{i\neq j}(u_j^{(k)}\cdot w_i^{(k)}) + X(k;\ell\ell',\ell''\ell)\sum_{i\neq j}(y_i^{(k)}\cdot\tilde{z}_j^{(k)})], \tag{16}$$

and

$$\tilde{g} = \sum_{k'}\left[X(k';\ell\ell',\ell\ell'')\sum_{i\neq j}(u_j^{(k')}\cdot\tilde{w}_i^{(k')}) + X(k';\ell\ell',\ell''\ell)\sum_{i\neq j}(\tilde{y}_i^{(k')}\cdot z_j^{(k')})\right]. \tag{17}$$

Upon substituting (16) and (17) into (5) we obtain after considerable manipulation

$$W_2 = W_A + W_B + W_C, \tag{18}$$

where

$$W_A = -\sum_{kk't} P(kk';\ell\ell',\ell\ell'')(2t+1)\begin{Bmatrix} kk't \\ \ell'\ell\ell''\end{Bmatrix}\cdot\sum_{ijs}[u_i^{(k')}\times(u_j^{(k)}\times v_s^{(t)})]^{(0)}, \tag{19}$$

$$W_B = -\sum_{kk't} P(kk';\ell\ell',\ell''\ell)(2t+1)\begin{Bmatrix} kk't \\ \ell'\ell\ell\end{Bmatrix}\begin{Bmatrix} kk't \\ \ell\ell\ell''\end{Bmatrix}\cdot\sum_{i\neq j}(u_i^{(t)}\cdot v_j^{(t)}), \tag{20}$$

$$W_C = -\sum_{kk't} Q(kk';\ell\ell',\ell\ell'')(2t+1)\begin{Bmatrix} kk't \\ \ell\ell'\ell''\end{Bmatrix}\cdot\Big\{\sum_{i\neq j\neq s}(-1)^{k+k'+t}[u_i^{(k)}\times \big([z_j^{(k')}\times\tilde{z}_s^{(t)}]^{(k)} + [z_j^{(t)}\times\tilde{z}_s^{(k')}]^{(k)}\big)]^{(0)} + 2\sum_{i\neq j}\begin{Bmatrix} kk't \\ \ell'\ell\ell\end{Bmatrix}(z_i^{(t)}\cdot\tilde{z}_j^{(t)})\Big\}, \tag{21}$$

$$Q(kk';\ell\ell',\ell\ell'') = X(k;\ell\ell',\ell\ell'')X(k';\ell\ell',\ell''\ell)/\Delta E. \tag{22}$$

W_B represents a two-body interaction and for even values of t is a linear combination of the coefficients of the Slater parameters $F_t(\ell\ell')$. However, new parameters are obtained for odd values of t. The second term of W_C, also representing a two-body interaction, yields new parameters with t equal to $\ell + \ell' + 1$. Hence a Hamiltonian $H^2_{\text{eff.}}$, containing the two-body contribution to W_2 may be written

$$H^2_{\text{eff.}} = -\sum_t F_t\sum_{i\neq j}(u_i^{(t)}\cdot v_j^{(t)}) - \sum_t G_t\sum_{i\neq j}(z_i^{(t)}\cdot\tilde{z}_j^{(t)}). \tag{23}$$

The two terms are referred to as the direct and exchange effective Slater parameters. The matrix elements of $H^2_{\text{eff.}}$ are diagonal in S and L, and are independent of J and M.

W_A represents a three-body interaction if $i \neq j \neq s$. Otherwise, it contains mixtures of one and two-body terms which either vanish or have been previously considered. Hence taking this term and the first term of

W_C, the Hamiltonian representing the three-body effective electrostatic direct and exchange interactions, may be written

$$H^3_{eff} = -\sum_{k'kt} \cup (k'kt) \sum_{i\neq j\neq s} [u_i^{(k')} \times u_j^{(k)} \times v_s^{(t)}]^{(0)} - \sum_{k'kt} V(k'kt) \sum_{i\neq j\neq s} (-1)^{k'+k+t} \cdot$$

$$[u_i^{(k)} \times \{(z_j^{(k')} \times \tilde{z}_s^{(t)})^{(k)} + (z_j^{(t)} \times \tilde{z}_s^{(k')})^{(k)}\}]. \tag{24}$$

The coefficients of F_t in the configuration d^n_p are found by calculating the matrix elements

$$(d^n(\alpha_1 S_1 L_1)p\,SLJM| \sum_{i\neq j} (u_i^{(t)} \cdot v_j^{(t)})| d^n(\alpha_1' S_1' L_1')p\,S'L'J'M').$$

Since this involves the reduced matrix element $(p\|v^{(t)}\|p)$, t may take only the values 0, 1 and 2 because of the triangular relationship $\delta(1,t,1)$ between the two p angular momenta and t. For t equal to 0 and 2 the Slater parameters F_0 and F_2 are included elsewhere (see sec. 3). Thus, the only new direct effective parameter for d^np as well as for $d^{n-1}sp$ and $d^{n-2}s^2p$ is F_1.

Similarly for G_t, the calculation of the matrix elements

$$(d^n(\alpha_1 S_1 L_1)p\,SLJM| \sum_{i\neq j} (z_i^{(t)} \cdot \tilde{z}_j^{(t)})| d^n(\alpha_1' S_1' L_1')p\,S'L'J'M')$$

is required. Due to the reduced matrix element $(d\|z^{(t)}\|p)$ with the triangular relation $\delta(2,t,1)$, t may take on the values 1, 2 or 3. Since G_1 and G_3 are already included elsewhere, the only new exchange effective parameter is G_2.

The three-body effective interactions involve 9 independent parameters. They were not included in this investigation as their contributions are not expected to be significant (see sec. 4).

3. Parameters

The algebraic matrices of $(d+s)^np$ comprise the electrostatic and spin orbit interaction matrices of the configurations d^np, $d^{n-1}sp$ and $d^{n-2}s^2p$; the electrostatic interactions between configurations $d^np - d^{n-1}sp$, $d^{n-1}sp - d^{n-2}s^2p$, $d^np - d^{n-2}s^2p$; the complete two and three-body effective interactions of the core d electrons, as well as two-body mixed effective interactions between the d and p electrons. The energy matrix (for a particular n) is then a linear combination of these matrices, the coefficients of which are parameters to be discussed below. Unprimed quantities denote the configuration d^np, primes denote $d^{n-1}sp$ and double primes denote $d^{n-2}s^2p$.

A, A', A''—the heights of the configurations,

$$S' = A' - A,\ S'' = A'' - A.$$

B, B', B''—linear combinations of the Slater parameters $F^2(d,d)$ and $F^4(d,d)$:

$$B = \frac{1}{441}[9F^2(dd) - 5F^4(dd)] = F_2(dd) - 5F_4(dd)\ ,\ [31].$$

C, C', C''—multiples of the Slater parameter $F^4(d,d)$:

$$C = \frac{5}{63} F^4(dd) = 35F_4(dd)\ ,\ [31].$$

G_{ds}—the parameter of the $d - s$ interaction in the configuration $d^{n-1}sp$:

$$G_{ds} = \frac{1}{5} G^2(ds)\ ,\ [22].$$

F_2, F_2', F_2''—parameters of the direct part of the d-p interaction:

$$F_2 = \frac{1}{35} F^2(dp) \text{ , [31].}$$

G_1, G_1', G_1''—parameters of the exchange part of the d-p interaction:

$$G_1 = \frac{1}{15} G^1(dp) \text{ , [31].}$$

G_3, G_3', G_3''—parameters of the exchange part of the d-p interaction:

$$G_3 = \frac{3}{245} G^3(dp) \text{ , [31].}$$

G_{ps}—the parameter of the $p-s$ interaction in the configuration $d^{n-1}sp$:

$$G_{ps} = \frac{1}{3} G^1(ps) \text{ , [32].}$$

H—the parameter of the $d^n - d^{n-1}s$ interaction:

$$H = \frac{R^2(dd,ds)}{35} \text{ , [22].}$$

H'—the parameter of the $d^{n-1}s - d^{n-2}s^2$ interaction, defined the same as H.

J—the parameter of the direct part of the $d^np - d^{n-1}sp$ interaction:

$$J = \frac{R^2(dp,sp)}{5} \text{ , [33].}$$

J'—the parameter of the direct part of the $d^{n-1}sp - d^{n-2}s^2p$ interaction, defined the same as J.

K—the parameter of the exchange part of the $d^np - d^{n-1}sp$ interaction:

$$K = \frac{R^1(dp,ps)}{3} \text{ , [33].}$$

K'—the parameter of the exchange part of the $d^{n-1}sp - d^{n-2}s^2p$ interaction, defined the same as K.

G^*—the parameter of the $d^np - d^{n-2}s^2p$ interaction:

$$G^* = \frac{R^2(dd,ss)}{5} \text{ , [22].}$$

The spin-orbit contribution to the Hamiltonian has the form (p. 120, TAS, [32],)

$$\sum_i \xi(r_i)\,(\ell_i \cdot s_i)$$

where r_i is the distance of the i th electron from the nucleus,

$$\xi(r_i) = \frac{1}{2\mu^2c^2} \frac{1}{r_i} \frac{\partial U(r_i)}{\partial r_i} \text{ , where}$$

$U(r_i)$ is the potential in which the i th electron moves and μ is the reduced mass of the electron. Then,

$$\zeta_{n\ell} = \hbar^2 \int_0^\infty R^2(n\ell)\xi(r)dr,$$

where $\frac{R(n\ell)}{r}$ is the radial part of the wave function. Then

ζ_d, ζ_d', ζ_d''—parameters of the spin-orbit interaction of the d-electrons.

ζ_p, ζ_p', ζ_p''—parameters of the spin-orbit interaction of the p-electron.

The following parameters were discussed in detail in the previous section:

α, α', α''—parameters of the $L(L+1)$ correction.
β, β', β''—parameters of the Q correction.
T, T', T'' parameters of the three-body effective
T_x, T_x', T_x'' interactions of the core d-electrons.
F_1, F_1', F_1''—parameters of the direct part of the effective interactions.
G_2, G_2', G_2''—parameters of the exchange part of the effective interactions.

The calculated Lande g-factors given by

$$g = \frac{3}{2} + \frac{S(S+1) - L(L+1)}{2J(J+1)}, \text{ [31]}$$

were also computed. Whenever observed g-values exist, they provide very useful information to help fit the experimental levels.

Racah and Shadmi [1,2,9] have shown that if $M(d^n)$, $M'(d^{n-1}s)$ and $M''(d^{n-2}s^2)$ are the centers of gravity of d^n, $d^{n-1}s$ and $d^{n-2}s^2$, i.e., the weighted averages of the terms of these configurations, then the parameters

$$D' = M'(d^{n-1}s) - M(d^n)$$

and

$$D'' = M''(d^{n-2}s^2) - M'(d^{n-1}s)$$

are linear functions with small quadratic corrections of n for the configurations $(3d+4s)^n$ in the second spectra of the iron group.

Now in d^np we must consider n interactions $d-p$, $n(n-1)/2$ interactions $d-d$. From page 200, TAS, [32], the center of gravity of dp is

$$M(dp) = F_0(dp) - (G_1 + \frac{7}{2}G_3). \tag{25}$$

From equation (78) of Racah [31], the center of gravity of d^2 is

$$M(d^2) = A + \frac{7}{9}(C-2B). \tag{26}$$

Also, (p.197, TAS, [32],)

$$M(ds) = F_0(ds) - \frac{G_{ds}}{2}, \tag{27}$$

$$M(ps) = F_0(ps) - \frac{F_{ps}}{2}. \tag{28}$$

Since H, H', J, J', K, K' and G^* don't have diagonal elements, they need not be considered for the centers of gravity.

Now, by taking into account α, we have

$$M(d^2) = A + \frac{7}{9}(C-2B) + \frac{32}{3}\alpha. \tag{29}$$

As explained in the previous section, the $L(L+1)$ correction has to be considered in the form $[L(L+1) - 6n]\,\alpha$. Thus, write

$$M(d^2) = A + \frac{7}{9}(C-2B) + 12\alpha - \frac{4}{3}\alpha. \tag{30}$$

For the βQ correction we note that since Q is a two-body operator, and for d^2 we have a contribution of 1/9, the net contribution to d^n will be $\frac{n(n-1)}{2}\left(\frac{1}{9}\right)$. Since T represents a three-body interaction, its contribution will involve a cubic in n. Since there is no interaction of s^2d^n with sd^{n+1} for $n = 0,9,10$, the polynomial must vanish for those n. For $n = 1$ the contribution is easily seen to be 70, and thus the contribution to d^n is (35/36) $n\,(9-n)\,(10-n)$. Directly from the algebraic matrices of the parameters T_x, T'_x and T''_x it was seen that these parameters do not contribute to the center of gravity.

Finally, the direct part of the effective interaction for d^np has no contribution to the center of gravity, whereas the exchange part gives nG_2.

Thus, we obtain

$$M(d^np) = A + \frac{7n(n-1)}{18}(C-2B) - n(G_1 + \frac{7}{2}G_3) + \frac{2n}{3}(10-n)\,\alpha + \frac{n(n-1)}{18}\beta + \frac{35}{36}n(9-n)(10-n)\,T + nG_2. \tag{31}$$

$$M'(d^{n-1}sp) = A' + \frac{7}{18}(n-1)(n-2)(C'-2B') - (n-1)(G'_1 + \frac{7}{2}G'_3) - \frac{(n-1)}{2}G_{d_s} - \frac{1}{2}G_{p_s} + \frac{2}{3}(n-1)(11-n)\,\alpha' + \frac{(n-1)(n-2)}{18}\beta' + \frac{35}{36}(n-1)(10-n)(11-n)\,T' + (n-1)G'_2. \tag{32}$$

Since for $d^{n-2}s^2p$ the interactions $d-s$ and $s-p$ are constant and thus can be incorporated into the height of the configuration, we have

$$M''(d^{n-2}s^2p) = A'' + \frac{7}{18}(n-2)(n-3)(C''-2B'') - (n-2)(G''_1 + \frac{7}{2}G''_3) - \frac{2}{3}(n-2)(12-n)\,\alpha'' + \frac{(n-2)(n-3)}{18}\beta'' + \frac{35}{36}(n-2)(11-n)(12-n)\,T'' + (n-2)\,G''_2. \tag{33}$$

The above expressions must be modified for complementary configurations ($n>5$). The matrices of B, C, α, and β for the configurations d^np, $d^{n-1}sp$, and $d^{n-2}s^2p$ are equal to the corresponding matrices of the complementary configurations $d^{10-n}s^2p$, $d^{11-n}sp$, and $d^{12-n}p$, respectively, [7]. Also, the matrices of G_{d_s} and G_{p_s} for $d^{n-1}sp$ are equal to the corresponding matrices of $d^{11-n}sp$. The matrices of T and G_2 must be replaced for complementary configurations by those of T_c and G_{2c}, respectively, [7]. Since the weighted average of the terms of d^9p is given by

$$M(d^9p) = M(d^9s^2p) = F_0 + (G_1 + \frac{7}{2}G_3),\ [32,\ \text{p. } 200]$$

we obtain

$$M(d^{12-n}p) = A + \frac{7}{18}(n-2)(n-3)(C-2B) + (n-2)(G_1 + \frac{7}{2}G_3) + \frac{2}{3}(n-2)(12-n)\alpha +$$

$$+ \frac{(n-2)(n-3)}{18}\beta + \frac{35}{36}(12-n)(n-2)(n-3)T_c + (12-n)G_{2c}. \quad (34)$$

$$M'(d^{11-n}sp) = A' + \frac{7}{18}(n-1)(n-2)(C'-2B') + (n-1)(G_1' + \frac{7}{2}G_3') - \frac{(n-1)}{2}G_{ds} -$$

$$- \frac{1}{2}G_{ps} + \frac{2}{3}(n-1)(11-n)\alpha' + \frac{(n-1)(n-2)}{18}\beta' + \frac{35}{36}(11-n)(n-1)(n-2)T_C' + (11-n)G_{2c}'. \quad (35)$$

$$M''(d^{10-2}s^2p) = A'' + \frac{7}{18}n(n-1)(C''-2B'') + n(G_1'' + \frac{7}{2}G_3'') + \frac{2}{3}n(10-n)\alpha'' +$$

$$+ \frac{n(n-1)}{18}\beta'' + \frac{35}{36}(10-n)n(n-1)T_c'' + (10-n)G_{2c}''. \quad (36)$$

The checks of the algebraic matrices were described previously by the author, [8,9]. In section 5, [9], we had

$$t + t_c + 160Q + 15L(L+1) - 80c = 240 - 40(n-2)(n-3). \quad (37)$$

In analogy to the above result we obtain

$$14t_x + 14t_{xc} - 1280Q - 15L(L+1) - 60b + 640c = 320n^2 - 1180n + k, \quad (38)$$

where

t, t_c, t_x, t_{xc}, b, and c are the algebraic matrices of the parameters T, T_c, T_x, T_{xc}, B, and C, respectively, and k is a numerical constant. The checks are possible because the sum of either t and t_c, or t_x and t_{xc}, gives rise only to two-body and one-body terms, that may be expressed as linear combinations of the algebraic matrices associated with the two and one-body parameters β, α, B, and C of the configuration d^n. The algebraic matrices of the parameters T, T', T'', T_c, T_c', T_c'', T_x, T_x', T_x'', T_{xc}, T_{xc}', and T_{xc}'' were added to the previously calculated matrices and the above checks utilized.

In the general treatment, with the exception of the centers of gravity $M(d^np)$, the parameters are *required* to satisfy the interpolation formula

$$P = P_0 + P_1(n-6) + P_2[(n-6)^2 - 10], \quad (39)$$

where P_0, P_1, and P_2 are the general parameters and replace the individual parameter P for all the spectra of the sequence; n is the number of $3d$ and $4s$ electrons for each spectrum. As an example, in table 42, B_0, B_0', B_0'' refer to the constant terms; B_1, B_1', B_1'' to the linear terms; B_2, B_2', B_2'' to effectively the quadratic terms, for the configurations d^np, $d^{n-1}sp$ and $d^{n-2}s^2p$, respectively, in the general treatment.

The above form of accounting for linearity with a quadratic correction, was chosen in order to make the parameters as nearly orthogonal as possible.

Since the parameter $M(d^np)$ incorporates setting the value of the lowest energy level to zero, it is not expected to behave regularly as a function of n. Consequently, when M, M', and M'' were replaced with

$$D' = M'(d^{n-1}sp) - M(d^np)$$

$$D'' = M''(d^{n-2}s^2p) - M'(d^{n-1}sp),$$

the latter were compelled to satisfy the relation (39).

4. Results

The source of the experimental data for all the elements with the exception of manganese is "Atomic Energy Levels", Vols. I and II by C.E. Moore, referred to as AEL, [35]. For manganese, the experimental results of Catalan, Meggers and Garcia-Riquelme, [36] were used. Details indicating the levels included, as well as those that were rejected, are provided in another paper, [17]. On fitting 1537 levels using 67 free interaction parameters a mean error of 182cm^{-1} was obtained. Altogether 3652 energy levels were calculated including all the levels for the configurations $3d^{n-2}4s^24p$ across the sequence.

Tables 1-41[2] yield the results for each of the parameters individually, whereas tables 42 and 43 give the results of the general interpolation formulas, together with the centers of gravity $M(d^np)$, $(0 \leqslant n \leqslant 10)$, $M_{11}(d^9s^2p)$ and $M_{12}(d^{10}s^2p)$, for the various significant stages of this project.

The error attributed to a parameter defines the range within which it may vary without the mean error increasing. In particular, if zero lies within the range of the value of a parameter and ± its error, then that particular parameter may be fixed at zero, which is equivalent to excluding it in the first place.

In this project, Hartree-Fock calculations were performed for all the configurations $3d^n4p$, $3d^{n-1}4s4p$ and $3d^{n-2}4s^24p$. Details of these calculations and results are given in another paper, [38].

With the exception of the results obtained from the Hartree-Fock calculations, the values of particular parameters pertaining to the three configurations $3d^n4p$, $3d^{n-1}4s4p$ and $3d^{n-2}4s^24p$ are in arithmetic progression, since there is insufficient experimental data for $3d^{n-2}4s^24p$ to determine parameters pertaining only to those configurations. Hence even in results arising from the least-squares computations these parameters do not have attached a ± error value. Furthermore, also in those cases where a parameter has a value in the least-squares either equal to the one directly preceding it (denoted, specifically, for the sake of clarity by *EQ.*), or if it is maintained at a fixed difference (unless specified otherwise, the differences that appears in the diagonalization, and denoted by F.D.), there is no ± error attached to the value of the parameter. In those cases where a parameter either changes sign or is ill-defined in the least-squares, it is fixed at either its value in the diagonalization, or at a value of zero (denoted by FIX). This procedure may also be followed if one is interested to study the effect of a particular parameter either on other parameters or in reducing the mean error, by considering two variations, one with the parameter left intact and in the other maintained at a value of zero.

The column PREVIOUS RESULTS refers to individual treatments without two- and three-body effective interactions, performed by the author for calcium-nickel, [10-16]. For the case of copper, the excellent results of Martin and Sugar, [38], for the configurations $3d^94s4p$ + $3d^84s^24p$ of CuI, were considered.

Results for the following parameters were obtained by the Hartree-Fock calculations: $B,B',B'',C,C',C'',F_2,F_2',F_2'',G_1,G_1',G_1'',G_3,G_3',G_3'',G_{ps},G_{ds},G^*,H,H',J,J',K,K',\zeta_d,\zeta_d',\zeta_d'',\zeta_p,\zeta_p'$, and ζ_p'' as indicated in Tables 3-32. Very interesting and important conclusions from these results, not known or anticipated previously, were that G^* is significantly larger than G_{ds}, whereas H' is appreciably smaller than H. The Hartree-Fock results for J' and K' in ZnI $3d^{10}4s4p$ + $3d^94s^24p$ were anomalous to the other values, and thus excluded from consideration.

All entries of the parameters are in cm^{-1}.

4.1 Initial values

These entries appear in DIAGON 1 in Tables 1-40, and in the column INITIAL in table 42 for the general interpolation parameters.

For the parameters D' and D'', least-squares optimization calculations were performed on those values obtained in the columns PREVIOUS RESULTS. Even when allowing for quadratic corrections, the deviations were quite large, especially near the center of the period, where the elements have the largest number of levels. Consequently, least-squares were performed, *weighing* the entry of each element proportionally to the number of its levels. When $(D')_2$ and $(D'')_2$, the quadratic corrections were allowed to be free, their values were very different with both assuming large errors. When they were restricted to be equal the common value was -87 ± 95. Consequently, initially D' and D'' were taken to be linear functions of the atomic

[2] All tables and figures are placed at the end of this paper, beginning on page 54.

number, as indicated in tables 1, 2, 42, and 43. Entries are given to two decimal places to ascertain that the interpolation relation, (39), for the parameters be satisfied.

From previous results obtained for the even configurations in the iron group by Racah, Shadmi, Oreg, Stein and Caspi, [1,2,28,29], and for the odd configurations by the author, [3,4], the parameters B and C behaved as linear functions of the atomic number.

For the parameters B,B', and B'' using the values obtained from the Hartree-Fock calculations, and demanding that they be in arithmetic progression, the best straight lines yielded

$$B = 976 + 84(n-6) \tag{40a}$$

$$B' = 1083 + 77(n-6) \tag{40b}$$

$$B'' = 1190 + 70(n-6). \tag{40c}$$

The Hartree-Fock results were on the average greater by a factor of 1.27 from the spectroscopic results. Hence the initial values given in tables 3-5, and 42 are the above values divided by 1.27.

Exactly as for the B,s, we obtain, using the Hartree-Fock results

$$C = 3558 + 310(n-6) \tag{41a}$$

$$C' = 3980 + 280(n-6) \tag{41b}$$

$$C'' = 4402 + 250(n-6). \tag{41c}$$

Again, the initial values for these parameters given in Tables 6-8, and 42 are the above values divided by the same factor of 1.27.

For F_2,F_2',F_2'' least-squares were performed on the Hartree-Fock results demanding that they be in arithmetic progression. When quadratic corrections were allowed, the mean error was 5.0cm^{-1}, with values of 1.2 $\pm$ 0.3cm^{-1} and 0.7 $\pm$0.2cm^{-1} for $(F_2)_2$ and $(F_2')_2$, respectively. When $(F_2)_2$ and $(F_2')_2$ were set equal, they had a common value of 1.0 $\pm$ 0.3cm^{-1}, with the mean error rising to 7.9cm^{-1}. When both were zero, the mean error only rose to 9.0cm^{-1}. Hence this variation was adopted, the parameters were restricted to be linear with initial values given in tables 9-11 and 42. However, the possibility of allowing for quadratic corrections in subsequent iterations and variations was permitted.

For the parameters G_1,G_1', and G_1'' when least-squares were performed on the Hartree-Fock results, the quadratic corrections were significant. When the parameters were forced to be linear, the mean error was 68 cm^{-1}, whereas with $(G_1)_2$ assuming a value of 7.8 $\pm$ 1.0cm^{-1} and $(G_1')_2$ a value of 3.5 $\pm$ 0.6cm^{-1} the mean error was reduced to 21 cm^{-1}. The initial values are given in tables 12-14 and 42. As for the F_2 parameters no scaling factor was used between the spectroscopic and the Hartree-Fock results.

From the definition of the G_3 parameters, it is clear that they should be allowed the same degree of freedom as the G_1 parameters. Hence the initial values given in tables 15-17 and 42, were obtained by allowing quadratic corrections in the least squares of the Hartree-Fock results, and then using a scale factor of 2 to divide the latter. This common factor was obtained by comparing the Hartree-Fock and spectroscopic results.

For the parameter G_{ps} the quadratic correction was very significant, reducing the mean error in the least-squares of the Hartree-Fock results from 79cm^{-1} to 27cm^{-1}. The values given in tables 18 and 42 are those obtained after dividing the least squares results by a common factor of 1.58.

For G_{ds} and G^*, least-squares calculations on the Hartree-Fock results decreased the value of the mean error from 91cm^{-1} to 38cm^{-1}, after allowing a quadratic correction. However, the values of $(G_{ds})_2$ and $(G^*)_2$ were sufficiently close to each other, 7.3 $\pm$ 1.5cm^{-1} and 8.9 $\pm$ 1.6cm^{-1}, respectively, that these were compelled to be equal in the initial computations. The latter were obtained by dividing the results from the least-squares by a common factor of 1.1.

For H and H', in the least-squares of the Hartee-Fock results, the values of H_1 and H_1' were -11.5 $\pm$ 1.6cm^{-1} and -13.5 $\pm$ 1.2cm^{-1}, respectively, whereas H_2 and H_2' were 2.9 $\pm$ 0.2cm^{-1} and 2.5 $\pm$ 0.2cm^{-1}, respectively. Consequently, both pairs of parameters were set equal. Then the mean error was only 5.8cm^{-1} and the results, without a scaling factor, are given in tables 21, 22, and 42.

Unlike the case of the H parameters, in the least-squares calculations of the Hartree-Fock results, J_1 and J_1' had to be different, as their values were $-28 \pm 8\text{cm}^{-1}$ and $14 \pm 7\text{cm}^{-1}$, respectively. However, J_2 and J_2'were sufficiently close to have a common value of $11 \pm 2\text{cm}^{-1}$. This quadratic correction was important in reducing the mean error from 98cm^{-1} to 41 cm^{-1}. The initial values in tables 23,24, and 42 are the least-square values divided by a common factor of 1.67 for both J and J'.

For K and K' the situation was very similar as that for J and J'—linearity with a common quadratic correction—here $24.5 \pm \text{cm}^{-1}$, yielded a mean error of 62cm^{-1} compared with 142cm^{-1}, when the parameters were forced to be linear. The initial values for K were obtained by using a scale factor of 1.28, whereas for K' the scale factor was 1.10. Hence, initally K_2 had a value of 19.15cm^{-1} and K_2', a value of 22.29cm^{-1} in the tables 25, 26 and 42.

In previous general treatments dealing with the spectra of the iron group [1-4,27,28], the parameters of the spin-orbit interaction generally required a quadratic correction. After performing several variations in the least-squares of the Hartree-Fock results, it was seen that the parameters $\zeta_d,\zeta_d',\zeta_d''$were required to have a quadratic correction, whereas the parameters ζ_p,ζ_p' and ζ_p'' could, initially, be linear.

The values of $(\zeta_d)_2$ and $(\zeta_d')_2$ in the least-squares of the Hartree-Fock results were $6.9 \pm 0.2\ \text{cm}^{-1}$ and $8.1 \pm 0.2\text{cm}^{-1}$, respectively. Hence they were set equal.

The mean error was then only 8.7cm^{-1}, reduced from 32cm^{-1} when the ζ_d parameters were linear. The values obtained from those least-squares calculations were used directly without a scaling factor and are given in Tables 60-62, and 75.

When least squares were performed on the Hartree-Fock results of ζ_p, ζ_p', and ζ_p'', demanding that they be in arithmetic progression, the value of $(\zeta_p)_2$ was $-0.2 \pm 0.3\text{cm}^{-1}$ and that of (ζ_p') was $0.3 \pm 0.2\text{cm}^{-1}$. Thus, these parameters were fixed at zero, and initially ζ_p, ζ_p', and ζ_p''were linear. Then, the mean error only increased from 7.9cm^{-1} to 8.2cm^{-1}. By comparing the Hartree-Fock and spectroscopic results, a common scale factor of 0.8 was used to divide the values of the least-squares, in order to obtain the initial values given in tables 30-32 and 42.

From the parameters of the effective interactions, previous values were available only for the α's. As this parameter behaved irregularly, a common average value of 60 was taken as the initial value of α, α', and α'' for all elements in the period. The initial values of β, β', β'', T, T', T'', T_x, T_x', T_x'', F_1, F_1', F_1'', G_2, G_2', and G_2'' were zero for all elements.

4.2 Preliminary iterations

For the general least-squares routine a maximum capacity for 101 parameters could be achieved.

In the first two iterations the parameters D', D'', G_1, G_1' G_3, $G_3'G_{ps}$ K, K', ζ_d, ζ_d', ζ_p, and ζ_p'were allowed independent quadratic variations as functions of the atomic number.

The parameters F_2, F_2' G_{ds}, G^*, H, H', J, and J' were permitted a quadratic variation with the restrictions

$$(F_2)_2 = (F_2')_2\ ,$$
$$(G_{ds})_2 = G_2^*\ ,$$
$$H_2 = H_2'\ ,$$
$$J_2 = J_2'\ .$$

The parameters B,B', C,C', α,α', F_1,F_1', G_2, and G_2'were allowed to vary linearly.

The parameters β,β', T,T', T_x, and T_x' varied linearly with the restrictions

$$\beta_1 = \beta_1'.$$
$$T_1 = T_1',$$
$$(T_x)_1 = (T_x')_1.$$

The remaining 13 places were reserved for the centers of gravity $M_0 - M_{12}$.

In the third iteration the restrictions

$$(G_{ds})_2 = G_2^*,$$
$$H_2 = H_2',$$
$$J_2 = J_2',$$

were not included. Thus, *all* the parameters for the interactions between configurations were permitted independent quadratic variations. The required places were obtained by realizing from the first two iterations that F_2 need vary only linearly and it was also possible to impose the restrictions

$$(G_1)_2 = (G_1')_2 \text{ and}$$
$$(G_3)_2 = (G_3')_2.$$

The initial parameters of the first variation are given in the column DIAGON 1, (tables 1-40), whereas the final values are given in the column GLS1, (table 42). These parameters, with some modifications, were used for the second iteration and given in the column DIAGON 2. The results of the most successful of many variations in the general least-squares are given in the column GLS2, which are essentially the ones used in the next iteration and given in the column DIAGON 3. Again the results of the best variation are given in the columns GLS3, and then used with some modifications for the next iteration.

The values of the least-squares where all 101 parameters are allowed to be free are given in the columns GLS 1a, GLS 2a, and GLS 3a.

From the results of GLS1a it is clear that we should have

$$D_2'' = D_2'$$
$$(F_2)_2 = 0 \text{ (FIX)}$$
$$(G_1')_2 = (G_1)_2 = 0 \text{ (FIX)}$$
$$(G_3')_2 = (G_3)_2$$
$$G_0^* - (G_{ds})_0 = 708 \text{ (F.D.)}$$
$$G_1^* = (G_{ds})_1$$
$$H_0 - H_0' = 34 \text{ (F.D.)}$$
$$K_2' = K_2$$
$$(\xi_d')_2 = (\xi_d)_2$$
$$(\xi_p')_1 = (\xi_p)_1$$
$$(\xi_p')_2 = (\xi_p)_2 = 0 \text{ (FIX)}$$
$$\alpha_0' = \alpha_0$$
$$\alpha_1' = \alpha_1$$
$$\beta_0' = \beta_0$$
$$T_0' = T_0$$
$$(T_x')_0 = (T_x)_0$$
$$(F_1')_0 = (F_1)_0$$
$$(F_1')_1 = (F_1)_1 = 0 \text{ (FIX)}$$
$$(G_2')_0 = (G_2)_0$$
$$(G_2')_1 = (G_2)_1,$$

which can be seen either directly from the results or by noting that otherwise the parameters are ill-defined. With the above restrictions there then remained 78 free parameters in that variation which was used for the next stage of the computations, GLS 1. In GLS 1, the sum of the squares of the deviations decreased from 2.83879×10^9 to 5.97895×10^7. Besides the changes in the M's, the parameter that had the greatest effect was C_1; while changing from 244 cm^{-1} to 408 $\pm$ 8cm^{-1} it reduced the sum of the squares of the deviations from 3.29325×10^8 to 2.57289×10^8.

In a variation where G_0^*, J_0', K_0' were free, but in addition to the restriction of GLS 1, there were the conditions

$$\begin{aligned} G_1^* &= (G_{ds})_1 \\ H_1' &= H_1 \\ J_1' &= J_1 \\ K_1' &= K_1 \end{aligned}$$

the parameters β_0, T_0, $(G_1')_2$, $(G_{ps})_2$, and H_2 were badly defined. In each case the ± error of the parameter exceeded its actual value.

In another variation, with the same restrictions as in GLS 1, but leaving β_1, $(F_1)_1$ and $(G_2')_0$ free, the values of these parameters were

$$\begin{aligned} \beta_1 &= -29 \pm 37 \\ (F_1)_1 &= 0.8 \pm 2.2 \\ (G_2')_0 &= 36 \pm 7. \end{aligned}$$

As $(G_2)_0$ had the value of 24 ± 8 it is clear that β_1 and $(F_1)_1$ should be zero whereas

$$(G_2)_0 = (G_2')_0.$$

In the second iteration when all 101 parameters are left free, GLS 2a, the G_3, F_1, and G_2 parameters behave erratically, whereas H_0', J_1', K_2', and $(\xi_d'')_2$ change sign. From these results and many other variations it became apparent that for the final variation in this iteration we should have

$$\begin{aligned} D_2'' &= D_2' \\ (F_2)_2 &= 0\,(\text{FIX}) \\ (G_1')_2 = (G_1)_2 &= 0\,(\text{FIX}) \\ (G_3')_0 &= (G_3)_0 \\ (G_3')_1 &= (G_3)_1 \\ (G_3')_2 = (G_3)_2 &= 0\,(\text{FIX}) \\ G_1^* &= (G_{ds})_1 \\ H_0 - H_0' &= 40\,(\text{F.D.}) \\ H_1' &= H_1 \\ J_1' &= J_1 \\ K_1' &= K_1 \\ K_2' &= K_2 \\ (\xi_d')_2 &= (\xi_d)_2 \\ (\xi_p')_2 &= (\xi_p)_2 \\ \alpha_0' &= \alpha_0 \\ \alpha_1' &= \alpha_1 \\ \beta_0' &= \beta_0 \\ T_0' &= T_0 \\ (T_x')_0 &= (T_x)_0 \\ (F_1')_0 &= (F_1)_0 \\ (F_1')_1 &= (F_1)_1 \\ (G_2')_1 &= (G_2)_1 \end{aligned}$$

with 77 free parameters remaining.

The sum of the squares of the deviations is decreased from 2.06466×10^8 to 5.71710×10^7. The parameters having the greatest effect were $(G_3)_0$, in changing from 27 cm^{-1} to 10 ± 1 cm^{-1} it reduced the sum of the deviations from 1.47723×10^8 to 1.14285×10^8; $(G_3)_1$ from -7 cm^{-1} to 2.2 ± 0.7 cm^{-1} and reduced $\sum_i(\Delta_i)^2$ from 1.14285×10^8 to 8.71367×10^7, and $(G_{ps})_2$, from 0 to -33 ± 5 cm^{-1}, and reduced $\sum_i(\Delta_i)^2$ from 5.97160×10^7 to 5.75448×10^7.

In the variation with parameters given in the column GLS 2*b*, the values of G_1^*, H_1', J_1', K_1', T_0', $(G_1)_2$, and $(G_3)_2$ are allowed to be free, whereas

$$\begin{aligned} G_0^* - (G_{ds})_0 &= 708\,(\text{F.D.}) \\ J_0' - J_0 &= 280\,(\text{F.D.}) \\ K_0' - K_0 &= 1020\,(\text{F.D.}). \end{aligned}$$

The results clearly show that G_1^* can't vary independently. H_1' and H_1 are too far apart with H_1' not well-defined. J_1 and J_1', as well as K_1 and K_1', have opposite signs, which is unacceptable. T_0' is well-defined but need not be different from T_0. Allowing $(G_1)_2$ and $(G_3)_2$ to vary has no significant effect. The reduction of the mean error from 203.1 cm^{-1} to 200.3 cm^{-1}, certainly does not justify allowing the increase in the number of parameters as then they do not behave reasonably.

In a variation identical to GLS 2, except that $D_2' \neq D_2''$, the values of these two parameters were -120 ± 5 cm^{-1} and -127 ± 11 cm^{-1}, respectively, showing clearly that they should be equal.

A variation in which G_1^*, H_1', J_1', K_1' are free, and all other conditions the same as in GLS 2, indicated that none of these parameters should be free, as they were either of different sign than the corresponding values G_1, H_1, J_1, and K_1, or were ill-defined.

In GLS 3a, with all 101 parameters free, the sum of the squares of the deviations was reduced from 9.62040×10^7 to 5.79187×10^7. However, several parameters such as G_0^*, G_1^*, G_2^*, H_0', J_0', J_1' and J_2' were badly defined.

From the results of GLS 3a, as well as many other variations wherein only a smal number of restrictions are imposed in each case, the following restrictions were imposed in the final variation of the third iteration, GLS 3, yielding 68 free parameters:

$$\begin{aligned} D_2'' &= D_2' \\ (F_2')_1 &= (F_2)_1 \\ (G_1')_1 &= (G_1)_1 \\ (G_1)_2 &= 0\,(\text{FIX}) \\ (G_3')_1 = (G_3)_1 &= 0\,(\text{FIX}) \\ (G_3)_2 &= 0\,(\text{FIX}) \\ G_1^* = (G_{ds})_1 &= -10\,(\text{FIX}) \\ G_2^* &= (G_{ds})_2 \\ H_0' &= 84\,(\text{FIX}) \\ H_1' &= \text{H}_1 \\ H_2' = H_2 &= 3\,(\text{FIX}) \\ J_1' &= J_1 \\ J_2' &= J_2 \\ K_1' &= K_1 \\ K_2' &= K_2 \\ (\xi_p')_1 &= (\xi_p)_1 \\ (\xi_p')_2 &= (\xi_p)_2 \\ (\xi_d')_2 &= (\xi_d)_2 \\ \alpha_0' &= \alpha_0 \\ \alpha_1' &= \alpha_1 \\ \beta_0' &= \beta_0 \\ T_0' &= T_0 \\ (T_x')_0 &= (T_x)_0 \\ (T_x)_1 &= -0.3\,(\text{FIX}) \\ (F_1')_0 &= (F_1)_0 \\ (F_1')_1 = (F_1)_1 &= 2\,(\text{FIX}) \\ (G_2')_0 &= (G_2)_0 \\ (G_2')_1 = (G_2)_1 &= 0\,(\text{FIX}) \end{aligned}$$

The sum of the squares of the deviations was reduced from 8.28089×10^7 to 5.12809×10^7. The only parameter that had a very significant effect was J_0, which changed from 1600 cm^{-1} to 1125 ± 39 cm^{-1}, thereby reducing the sum of the squares of the deviations from 7.63469×10^7 to 6.39959×10^7. Although all the parameters had reasonable well-defined values, the change in the sum of the squares of the deviations was such that a further iteration was required.

In GLS 3b, there are 76 free parameters. The same conditions apply as for GLS 3a, with the exception of $(F_2')_1$, $(\xi_p')_1$, $(T_z)_1$, $(F_1)_1$, $(G_2)_1$ being free; $G_1^* = (G_{ds})_1$, but not fixed at -10 cm^{-1}; $(G_3')_1 = (G_3)_1$, but not fixed at 0; $H_2' = H_2$, but not fixed at 3 cm^{-1}.

Although the parameters are very reasonable, the mean error actually increased from 196.7 cm^{-1} to 198.1 cm^{-1}, indicating that the improvement caused by these parameters was more than counterbalanced by the fact that their number increased.

In GLS 3c there are 72 free parameters. The same conditions apply as for GLS 3a, with the exception of H_0', K_1', and $(F_1)_1$ being free; $G_1^* = (G_{ds})_1$, but not forced at -10 cm^{-1}. Although the mean error decreases to 194.5 cm^{-1}, the parameters K_1' and $(F_1)_1$ change sign, while the value of 51 ± 12 cm^{-1} is definitely too small for H_0'.

In a variation where J_1' was allowed to vary freely, although its value changed from 50 cm^{-1} to the unreasonable value of -304 ± 44 cm^{-1}, the sum of the squares of the deviations only decreased as a consequence from 6.74632×10^7 to 6.67194×10^7. Furthermore, such a value for J_1' would cause J' to become negative for Cu I. Clearly, then J_1' should equal J_1 as in GLS 3.

In a variation where D_2' was not equal D_2'' and $(F_1)_0$ not equal to $(F_1')_0$, the resulting values were

$$\begin{aligned} D_2' &= -117 \pm 5 \text{ cm}^{-1} \\ D_2'' &= -109 \pm 11 \text{ cm}^{-1} \\ (F_1)_0 &= -13 \pm 6 \text{ cm}^{-1} \\ (F_1')_0 &= -9 \pm 6 \text{ cm}^{-1}, \end{aligned}$$

and thus as in GLS 3 these parameters should be respectively equal to each other.

The values of the parameters of the individual least squares of the third iteration are given in tables 3–40.

4.3. Final iteration.

For this iteration the 101 places for the parameters were the same as for the previous iteration.

From the final results of that iteration, GLS 3, as well as several different variations in this iteration, it became evident that 67 parameters should be free in the final results, GLS 4. Thus, the following 34 restrictions were imposed:

$$\begin{aligned} D_2'' &= D_2' \\ (F_2')_1 &= (F_2)_1 \\ (G_1')_1 &= (G_1)_1 \\ (G_1)_2 &= 0 \text{ (FIX)} \\ (G_3')_1 = (G_3)_1 &= 0 \text{ (FIX)} \\ (G_3)_2 &= 0 \text{ (FIX)} \\ G_0^* - (G_{ds})_0 &= 231 \text{ (F.D.)} \\ G_1^* = (G_{ds})_1 &= 0 \text{ (FIX)} \\ G_2^* &= (G_{ds})_2 \\ H_0' &= 84 \text{ (FIX)} \\ H_1' &= H_1 \\ H_2' = H_2 &= 0 \text{ (FIX)} \\ J_1' &= J_1 \\ J_2' &= J_2 \\ K_1' &= K_1 \\ K_2' &= K_2 \\ (\xi_p')_1 &= (\xi_p)_1 \end{aligned}$$

$$
\begin{aligned}
(\zeta_p')_2 &= (\zeta_p)_2 \\
(\zeta_d')_2 &= (\zeta_d)_2 \\
\alpha_0' &= \alpha_0 \\
\alpha_1' &= \alpha_1 \\
\beta_0' &= \beta_0 \\
T_0' &= T_0 \\
(T_x')_0 &= (T_x)_0 \\
(T_x)_1 &= 0\,(\text{FIX}) \\
(F_1')_0 &= (F_1)_0 \\
(F_1')_1 &= (F_1)_1 = 0\,(\text{FIX}) \\
(G_2')_0 &= (G_2)_0 \\
(G_2')_1 &= (G_2)_1 = 0\,(\text{FIX}).
\end{aligned}
$$

Hence in the final results the parameters D', D'', G_{ps}, G_{ds}, G^*, J, J', K, K', ζ_d, ζ_d', ζ_d'', ζ_p, ζ_p', and ζ_p'' required quadratic corrections, with the restrictions noted above. In particular, G_{ds} and G^* did not have linear terms. All the other parameters were linear functions of the atomic number. Furthermore, T_x, T_x', T_x'', F_1, F_1', F_1'', G_2, G_2', and G_2'' were constant for all spectra across the entire period.

The sum of the squares of the deviations only decreased from 5.83692×10^7 to 4.87994×10^7 for all the parameters. In *each* case the change in a parameter from the value in the diagonalization to its value in the least squares was less than the statistical error associated with the parameter. All the parameters have very reasonable values and are well-defined. The comparisons between these final results and those obtained from the Hartree-Fock calculations as well as those of previous results, are indicated graphically at the end of this section.

In GLS4a, where all the 101 parameters are free, although the mean error is only 171.3cm^{-1}, the parameters are not nearly as well defined as those of GLS4. Furthermore, the values of J_0' at $598 \pm 271\text{cm}^{-1}$, J_1' at $-376 \pm 127\ \text{cm}^{-1}$, $(F_1')_1$ at $-11 \pm 4\text{cm}^{-1}$, $(F_1'')_1$ at -20cm^{-1} (causing both F' and F'' to assume positive and negative values for different elements of the period), are not reasonable.

In GLS4b, the parameter G_0^* is allowed to be free and changes from 1820cm^{-1} to a value of $1649 \pm 83\text{cm}^{-1}$, thereby decreasing the sum of the squares of the deviations only from 5.40826×10^7 to 5.38969×10^7. Hence G^* is then uniformly higher than G_{ds} by only 56cm^{-1}. Thus, the significant difference between G^* and G_{ds} obtained in the Hartree-Fock calculations and the initial iterations becomes considerably less pronounced here. Nevertheless, in view of the other considerations above, G_0^* was maintained in the final variation at 1826cm^{-1}, a fixed difference of 231cm^{-1} above the value of $(G_{ds})_0$.

In GLS4c, there are 71 free parameters, the same restrictions are imposed as in GLS4, with the exception that G_0^*, H_0', J_1', and $(F_1)_1$ are left free. Although the mean error is reduced from 182.2cm^{-1} to 176.1cm^{-1} and the values for G_0^* of $1674 \pm 81\text{cm}^{-1}$ and $(F_1)_1$ of $-4 \pm 2\text{cm}^{-1}$ are reasonable, the value for H_0' of $42 \pm 15\ \text{cm}^{-1}$ is much too low, whereas the value for J_1' of $-231 \pm 37\ \text{cm}^{-1}$ is definitely unacceptable.

In another variation, with the same restrictions as in GLS4, but $(F_1)_1$ free, the value of this parameter was $-5 \pm 2\text{cm}^{-1}$. Coupled with a value of $(F_1)_0$ of $-11 \pm 4\text{cm}^{-1}$, the parameter F_1 assumes negative and positive values for different spectra of the period, which is unacceptable.

In GLS4d, the following additional 26 levels, which although having deviations exceeding the maximum tolerated for the other iterations ($\sim 600\text{cm}^{-1}$), had deviations below 1000cm^{-1} when inserted into the least squares.

Ti

1. The level $3d^24s(b^2P)4py^3S$ at $35439.43\ \text{cm}^{-1}$.
2. The three levels $3d^3(a^2G)4pt^3F_{2,3,4}$ at 38451.29cm^{-1}, 38544.38cm^{-1} and 38670.73cm^{-1}.
3. The level $3d^3(a^2G)4px^1G$ at 38959.53cm^{-1}.
4. The level $3d^3(a^2P)4pw^1D$ at 39265.80cm^{-1}.
5. The three levels $3d^3(a^2P)4pr^3D$ at 40556.70cm^{-1}, 40670.60cm^{-1}, and 40844.19cm^{-1}.

V

1. The level 1° at 34019.12cm^{-1}.
2. The four levels of $3d^4(a^3G)4pt^4F$ at 41389.49cm^{-1}, 41428.93cm^{-1}, 41492.29cm^{-1}, and 41599.36cm^{-1}.

Cr

1. The level $3d^4 4s(a^2P)4px^3S$ at 60084.09cm^{-1}.

Mn

1. The four levels $3d^6(^3G)4pw^4H$ at 63395.45cm^{-1}, 63444.61cm^{-1}, 63457.85cm^{-1}, and 63363.54cm^{-1}.

Fe

1. The five levels $3d^4 4s(a^4D)4px^5D$ at 39625.829cm^{-1}, 39969.880cm^{-1}, 40231.365cm^{-1}, 40404.544cm^{-1}, and 40491.32cm^{-1}.

Cu

1. The two levels $3d^9 4s(^1D)4p''\ ^2P$ at 56343.74cm^{-1} and 58364.73cm^{-1}.

The restrictions are the same as in the case of GLS4, and as expected, the parameters are well-defined and reasonable. However, the mean error increases substantially from 182.2cm^{-1} to 199.7cm^{-1}.

In GLS4e there are 65 parameters. In addition to the restrictions of GLS4, the conditions

$$(F_1)_0 = (F_1')_0 = (F_1'')_0 = 0(\text{FIX})$$

$$(G_2)_0 = (G_2')_0 = (G_2'')_0 = 0(\text{FIX})$$

are imposed. As a consequence, the parameters of the two-body effective interactions $d-p$: F_1, F_1', F_1'', G_2, G_2', and G_2'' are eliminated. Surprisingly, the mean error only increases from 182.2cm^{-1} to 183.5cm^{-1}. The elimination of these parameters also affects very slightly the values of the other parameters, and thus their overall effects are minimal indeed. Consequently, the higher order three-body effective interactions $d-p$ were not included (see the end of sec. 2).

In the variation GLS4f, there are 64 free parameters. In addition to the elimination of the F_1 and G_2 parameters, as in GLS4e, the condition

$$(T_x)_0 = (T_x')_0 = (T_x'')_0 = 0(\text{FIX})$$

was imposed. Hence the three-body effective interaction parameters of the d-electrons, T_x, T_x', and T_x'' were eliminated. The mean error rose to 189.1cm^{-1}, indicating that the T_x parameters have a considerably greater effect than the F_2 and G_1 parameters combined. The significant increase in the value of

$$\beta_0 = \beta_0' = \beta_0''$$

from -527 ± 28cm^{-1} in GLS4 to the present value of -673 ± 31cm^{-1}, should be noted.

In GLS4g, there are 62 parameters. In addition to the elimination of the F_1, G_2, and T_x parameters, as in GLSf, the conditions

$$T_0 = T_0' = T_0'' = 0(\text{FIX})$$

$$T_1 = T_1' = T_1'' = 0(\text{FIX})$$

are imposed. Hence both parameters of the effective interactions of the d-electrons are eliminated. As expected, the effects here are very pronounced, the mean error rising from 189.1cm^{-1} to 203.7cm^{-1}. Thus the effect of T is twice as great as T_x, and 11 times as large as F_2 and G_1 combined! As expected, the elimination of T has profound effects on the other remaining effective intersection parameters:

$$\alpha_0 = \alpha_1' = \alpha_0''$$

increases from 30 ± 3cm^{-1} to 61 ± 2cm^{-1}, whereas

$$\beta_0 = \beta_0' = \beta_0''$$

changes from $-673 \pm 31\,\mathrm{cm}^{-1}$ to $-336 \pm 32\,\mathrm{cm}^{-1}$.

In GLS 4h there are also 62 free parameters. The F_2 and G_1 parameters are included, but instead the restrictions

$$\beta_0 = \beta_0' = \beta_0'' = 0(\mathrm{FIX})$$

$$\beta_1 = \beta_1' \quad \beta_1'' = 0(\mathrm{FIX})$$

are imposed.

Hence, β, β', and β'' are eliminated. The results again deteriorate, the mean error rising from $203.7\mathrm{cm}^{-1}$ to $210.8\mathrm{cm}^{-1}$. As expected, the F_1 and G_2 parameters have similar values as in GLS4 and GLS4d.

$$\alpha_0 = \alpha_0' = \alpha_0''$$

has the higher value of $71 \pm 1\,\mathrm{cm}^{-1}$, incorporating partially the other effective parameters.

In GLS4i, there are only 60 free parameters. Here, in addition to the restrictions of GLS4, the parameters β, β', β'', $T, T', T'', T_x, T_x', T_x''$, F_1, F_1', F_1'', G_2, G_2' and G_2'' are eliminated. The mean error rises to $211.4\mathrm{cm}^{-1}$. Comparing this value with that of GLS4h (Δ of $210.8\mathrm{cm}^{-1}$) emphasizes again the minimal effects of the parameters F_2 and G_1. α_0 again has the high value of $72 \pm 1\mathrm{cm}^{-1}$.

In conclusion, starting from the 67 parameters in GLS4, the elimination of F_2 and G_1 increases the mean error by only $1.3\mathrm{cm}^{-1}$, T_x by a further $5.6\mathrm{cm}^{-1}$, T by an additional $14.6\mathrm{cm}^{-1}$, and β by an additional $7.7\mathrm{cm}^{-1}$.

The values of the parameters of the individual least squares of the final iteration are given in tables 3–40. More detailed discussions of the individual least squares are given in the paper dealing with the correspondence of the energy levels of the various configurations $(3d+4s)^n 4p$, [17].

4.4 Plots of parameters

Figures 1–17 describe graphically the variation of the parameters as functions of the atomic number for the cases of the previous results, Hartree-Fock computations and the final general least-squares (GLS4). In the case of the previous results, PR, the entries are from individual least squares and are indicated by a dot, •; whenever a particular parameter varied freely the ± value of the error is also given. For the case of Hartree-Fock computations, HF, the entries are given by a solid triangle, ▲; whereas a solid square, ■, denotes the results of the final GLS.

Since T_x, T_x', T_x'', F_1, F_1', F_1'', G_2, G_2', G_2'' are constant in the final results, their graphs clearly need not be drawn. Graphs of all the other parameters are given.

The sets of parameters B, B', B''; C, C', C''; F_2, F_2', F_2''; G_1, G_1', G_1''; G_3, G_3', G_3''; $\zeta_d, \zeta_d', \zeta_d''$; $\zeta_p, \zeta_p', \zeta_p''$; are in arithmetic progression in the least squares. Consequently, in order to indicate explicitly this interdependence, separate graphs were drawn where each set of three parameters appears together.

The graphs vividly illustrate and contrast the often irregular behavior of the parameters in the previous results, with the smooth, regular and very reasonable variations obtained in the present project for both the Hartree-Fock computations and, of course, for the general least squares. The contrasts are particularly prominent for the parameters of the interactions between configurations. There is general qualitative agreement between the Hartree-Fock results and those of the GLS. The only notable exceptions are the parameters F_2, F_2', and F_2'', as they increase slowly in the GLS as functions of the atomic number, whereas in the Hartree-Fock computations they decrease.

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TABLE 1. *Results for the parameter D'*

El.	Previous results	DIAGON 1	DIAGON 2	DIAGON 3	DIAGON 4	Final GLS
Ca	−18902	−17851.26	−19140	−19497	−19247	−19252
Sc	−14492	−13958.87	−14420	−14681	−14506	−14525
Ti	−10511	−10066.48	−9940	−10119	−9999	−10026
V	−5504	−6174.09	−5700	−5811	−5726	−5755
Cr	−2275	−2281.70	−1700	−1757	−1687	−1712
Mn	1554	1610.69	2060	2043	2118	2103
Fe	6185	5503.08	5580	5589	5689	5690
Co	8939	9395.47	8860	8881	9026	9049
Ni	12367	13287.85	11900	11919	12129	12180
Cu		17180.24	14700	14703	14998	15083

TABLE 2. *Results for the parameter D"*

El.	Previous results	DIAGON 1	DIAGON 2	DIAGON 3	DIAGON 4	Final GLS
Sc	4833	4817.60	4880	5140	5028	4950
Ti	12010	10768.97	11440	11740	11585	11532
V	17228	16720.34	17760	18086	17908	17886
Cr	20565	22671.71	23840	24178	23997	24012
Mn	27138	28623.08	29680	30016	29852	29910
Fe	36419	34574.45	35280	35600	35473	35580
Co	41960	40525.82	40640	40930	40860	41022
Ni	47690	46477.18	45760	46006	46013	46236
Cu	51395	52428.55	50640	50828	50932	51222
Zn		58379.92	55280	55396	55617	55980

TABLE 3. *Results for the parameter B*

El.	Previous results	Hartree-Fock	DIAGON 1	DIAGON 2	DIAGON 3	DIAGON 4	ILS 3	Final ILS	Final GLS
Sc	529±6	615.95	501	526	515	509	536±7	518±4	510
Ti	554±7	724.20	568	578	568	561	555±6	549±6	561
V	579±12	816.61	635	630	621	613	547±12	570±10	612
Cr	677±7	900.84	702	682	674	665	652±8	666±7	663
Mn	800±14	980.13	769	734	727	717	722±15	739±14	714
Fe	738±9	1056.03	836	786	780	769	768±11	759±4	765
Co	833±8	1129.51	903	838	833	821	841±16	842±10	816

TABLE 4. *Results for the parameter B'*

El.	Previous results	Hartree-Fock	DIAGON 1	DIAGON 2	DIAGON 3	DIAGON 4	ILS 3	Final ILS	Final GLS
Ti	651±7	850.52	670	677	669	665	655±7	655±6	664
V	730±5	934.80	731	739	729	726	723±6	715±5	724
Cr	755±5	1013.87	792	801	789	787	769±8	776±7	784
Mn	861±4	1089.50	853	863	849	848	843±6	843±7	844
Fe	943±7	1162.72	914	925	909	909	901±5	904±3	904
Co	956±6	1234.15	975	987	969	970	983±10	1001±12	964
Ni	1024±7	1304.17	1036	1049	1029	1031	1021±7	1017±7	1024

TABLE 5. *Results for the parameter B"*

El.	Previous results	Hartree-Fock	DIAGON 1	DIAGON 2	DIAGON 3	DIAGON 4	ILS 3	Final ILS	Final GLS
V	881	1041.24	827	848	837	839	899	860	833
Cr	833	1116.47	882	920	904	909	886	886	903
Mn	922	1189.31	937	992	971	979	964	948	973
Fe	1148	1260.59	992	1064	1038	1049	1034	1049	1043
Co	1079	1330.49	1047	1136	1105	1119	1135	1160	1113
Ni	1109 (FIX)	1399.33	1102	1208	1172	1189	1164	1175	1183
Cu	1000 (FIX)	1467.33	1157	1280	1239	1259	1239 (FIX)	1259 (FIX)	1253

TABLE 6. *Results for the parameter C*

El.	Previous results	Hartree-Fock	DIAGON 1	DIAGON 2	DIAGON 3	DIAGON 4	ILS 3	Final ILS	Final GLS
Sc	714±69	2221.17	1826	1266	1222	1240	762±69	866±47	1281
Ti	1661±33	2623.15	2070	1674	1655	1677	1741±31	1747±30	1714
V	2084±23	2965.90	2314	2082	2088	2114	2204±42	2228±38	2147
Cr	2445±15	3277.50	2558	2490	2521	2551	2596±51	2535±48	2580
Mn	2772±17	3569.86	2802	2898	2954	2988	3121±71	3108±63	3013
Fe	3310±29	3849.30	3046	3306	3387	3425	3404±31	3435±25	3446
Co	3744±63	4119.39	3290	3714	3820	3862	3852±84	3797±70	3879

TABLE 7. *Results for the parameter C'.*

El.	Previous results	Hartree-Fock	DIAGON 1	DIAGON 2	DIAGON 3	DIAGON 4	ILS 3	Final ILS	Final GLS
Ti	2319±57	3131.03	2473	2343	2257	2285	2380±38	2354±38	2318
V	2587±19	3443.16	2693	2647	2611	2636	2658±29	2722±30	2666
Cr	2918±12	3735.06	2913	2951	2965	2987	3029±39	2999±37	3014
Mn	3140±9	4013.59	3133	3255	3319	3338	3410±57	3413±50	3362
Fe	3509±14	4282.74	3353	3559	3673	3689	3687±18	3688±16	3710
Co	3875±18	4545.00	3573	3863	4027	4040	3994±35	3954±34	4058
Ni	4187±54	4801.79	3793	4167	4381	4391	4394±45	4439±43	4406

TABLE 8. *Results for the parameter C"*

El.	Previous results	Hartree-Fock	DIAGON 1	DIAGON 2	DIAGON 3	DIAGON 4	ILS 3	Final ILS	Final GLS
V	3090	3878.88	3072	3212	3134	3158	3112	3216	3185
Cr	3391	4155.83	3268	3412	3409	3423	3462	3463	3448
Mn	3508	4423.76	3464	3612	3684	3688	3699	3718	3711
Fe	3708	4685.03	3660	3812	3959	3953	3970	3940	3974
Co	4006	4941.20	3856	4012	4234	4218	4136	4111	4237
Ni	4287	5193.31	4052	4212	4509	4483	4522	4531	4500
Cu	4500 (FIX)	5442.15	4248	4412	4784	4748	4784 (FIX)	4748 (FIX)	4763

TABLE 9. *Results for the parameter F_2*

El.	Previous results	Hartree-Fock	DIAGON 1	DIAGON 2	DIAGON 3	DIAGON 4	ILS 3	Final ILS	Final GLS
Ca	128±2	306.13	273.34	200	151	178	171±24	190±27	170.5
Sc	201±8	258.97	259.70	200	156	180	212±9	200±11	173
Ti	153±9	235.96	246.05	200	161	182	163±6	167±5	175.5
V	160±8	220.50	232.40	200	166	184	182±7	168±6	178
Cr	187±10	208.61	218.75	200	171	186	196±8	189±5	180.5
Mn	193±7	198.79	205.10	200	176	188	206±9	178±8	183
Fe	173±10	190.32	191.45	200	181	190	205±7	202±7	185.5
Co	218±10	182.79	177.80	200	186	192	221±10	226±9	188
Ni	166±13	175.92	164.15	200	191	194	167±21	170±15	190.5

TABLE 10. *Results for the parameter* F_2'

El.	Previous results	Hartree-Fock	DIAGON 1	DIAGON 2	DIAGON 3	DIAGON 4	ILS 3	Final ILS	Final GLS
Sc	284±8	300.16	305.77	300	279	291	297±11	285±12	289
Ti	286±8	290.88	298.09	300	281.5	293	318±5	317±5	291.5
V	282±6	283.55	290.41	300	284	295	286±6	274±6	294
Cr	275±5	277.22	282.73	300	286.5	297	287±5	297±5	296.5
Mn	314±4	271.46	275.06	300	289	299	308±10	290±10	299
Fe	305±5	266.08	267.38	300	291.5	301	315±4	322±5	301.5
Co	303±7	260.91	259.70	300	294	303	305±8	311±7	304
Ni	311±7	255.92	252.02	300	269.5	305	300±9	304±8	306.5
Cu	329±12	251.02	244.35	300	299	307	319±7	319±9	309

TABLE 11. *Results for the parameter* F_2''

El.	Previous results	Hartree-Fock	DIAGON 1	DIAGON 2	DIAGON 3	DIAGON 4	ILS 3	Final ILS	Final GLS
Ti	419	354.97	350.13	400	402	404	473	468	407.5
V	404	352.41	348.42	400	402	406	390	380	410
Cr	363	349.86	346.71	400	402	408	378	405	412.5
Mn	435	347.26	345.01	400	402	410	410	402	415
Fe	437	344.57	343.31	400	402	412	425	442	417.5
Co	388	341.77	341.60	400	402	414	389	396	420
Ni	456	338.86	339.89	400	402	416	433	434	422.5
Cu	480 (FIX)	335.82	338.18	400	402	418	422	432	425
Zn		332.70		400	402	420			427.5

TABLE 12. *Results for the parameter* G_1

El.	Previous results	Hartree-Fock	DIAGON 1	DIAGON 2	DIAGON 3	DIAGON 4	ILS 3	Final ILS	Final GLS
Ca	394±2	559.20	501.60	231	305	328	419±29	423±32	327.5
Sc	335±9	367.63	405.13	226	289	309	344±10	347±11	309
Ti	283±10	290.99	324.32	221	273	290	287±5	288±5	290.5
V	229±8	247.17	259.17	216	257	271	251±7	251±7	272
Cr	224±7	217.86	209.69	211	241	252	243±8	241±7	253.5
Mn	227±7	196.41	175.88	206	225	233	220±8	230±9	235
Fe	202±8	179.74	157.73	201	209	214	237±7	238±5	216.5
Co	196±9	166.21	155.25	196	193	195	199±9	199±10	198
Ni	165±9	154.84	168.43	191	177	176	172±11	171±10	179.5

TABLE 13. *Results for the parameter* G_1'

El.	Previous results	Hartree-Fock	DIAGON 1	DIAGON 2	DIAGON 3	DIAGON 4	ILS 3	Final ILS	Final GLS
Sc	327±12	328.91	349.14	330	323	336	354±13	344±16	335
Ti	288±10	293.92	309.30	311	307	317	328±6	325±6	316.5
V	281±8	271.04	276.55	292	291	298	301±6	294±7	298
Cr	236±5	254.27	250.87	273	275	279	239±7	262±5	279.5
Mn	245±6	241.08	232.26	254	259	260	232±9	247±8	261
Fe	245±7	230.18	220.73	235	243	241	248±6	255±5	242.5
Co	199±7	220.78	216.28	216	227	222	210±8	213±7	224
Ni	223±9	212.51	218.90	197	211	203	227±12	226±12	205.5
Cu	284±2	205.00	228.59	178	195	184	206±13	208±16	187

TABLE 14. *Results for the parameter* G_1''

El.	Previous results	Hartree-Fock	DIAGON 1	DIAGON 2	DIAGON 3	DIAGON 4	ILS 3	Final ILS	Final GLS
Ti	293	311.36	294.28	401	341	344	369	362	342.5
V	333	300.52	293.93	368	325	325	351	337	324
Cr	248	292.02	292.05	335	309	306	235	283	305.5
Mn	263	284.95	288.64	302	293	287	244	264	287
Fe	288	278.81	283.73	269	277	268	259	272	268.5
Co	202	273.28	277.31	236	261	249	221	227	250
Ni	281	268.19	269.37	203	245	230	282	281	231.5
Cu	284 (EQ.)	263.39	259.91	170	229	211	240	235	213
Zn		258.81	248.94	137	213	192			194.5

TABLE 15. *Results for the parameter* G_3

El.	Previous results	Hartree-Fock	DIAGON 1	DIAGON 2	DIAGON 3	DIAGON 4	ILS 3	Final ILS	Final GLS
Ca	0 (FIX)	66.67	30.42	62	5	15	5 (FIX)	15 (FIX)	13
Sc	5±3	45.84	24.96	55	5	15	8±6	4±5	13
Ti	10±3	37.21	20.38	48	5	15	8±3	7±3	13
V	13±2	32.11	16.67	41	5	15	18±3	14±3	13
Cr	16±1	28.61	13.82	34	5	15	10±3	7±2	13
Mn	18±1	25.98	11.85	27	5	15	24±3	14±3	13
Fe	20±2	23.90	10.75	20	5	15	17±3	18±2	13
Co	14±2	22.18	10.52	13	5	15	13±4	13±3	13
Ni	14±4	20.70	11.16	6	5	15	7±5	6±5	13

TABLE 16. *Results for the parameter* G_3'

El.	Previous results	Hartree-Fock	DIAGON 1	DIAGON 2	DIAGON 3	DIAGON 4	ILS 3	Final ILS	Final GLS
Sc	5 (EQ.)	45.63	24.04	60	15	23	18±6	4 (EQ.)	21
Ti	10 (EQ.)	41.50	21.68	53	15	23	21±3	22±3	21
V	13 (EQ.)	38.66	19.72	46	15	23	24±3	17±3	21
Cr	16 (EQ.)	36.50	18.16	39	15	23	29±3	30±2	21
Mn	18 (EQ.)	34.73	16.99	32	15	23	30±4	22±4	21
Fe	20 (EQ.)	33.23	16.21	25	15	23	20±2	21±4	21
Co	14 (EQ.)	31.90	15.82	18	15	23	14±3	15±2	21
Ni	14 (EQ.)	30.71	15.84	11	15	23	11±6	12±6	21
Cu	51±1	29.62	16.24	4	15	23	31±6	35±7	21

TABLE 17. *Results for the parameter* G_3''

El.	Previous results	Hartree-Fock	DIAGON 1	DIAGON 2	DIAGON 3	DIAGON 4	ILS 3	Final ILS	Final GLS
Ti	10	47.75	22.98	58	25	31	34	37	29
V	13	46.23	22.77	51	25	31	30	20	29
Cr	16	44.98	22.49	44	25	31	48	53	29
Mn	18	43.89	22.12	37	25	31	36	30	29
Fe	20	42.90	21.67	30	25	31	23	24	29
Co	14	42.00	21.13	23	25	31	15	17	29
Ni	14	41.14	20.52	16	25	31	15	18	29
Cu	51 (EQ.)	40.32	19.82	9	25	31	41	43	29
Zn		39.53	19.03	2	25	31			29

TABLE 18. *Results for the parameter G_{ps}*

El.	Previous results	Hartree-Fock	DIAGON 1	DIAGON 2	DIAGON 3	DIAGON 4	ILS 3	Final ILS	Final GLS
Ca	4977±19	8451.47	5384.41	5326	4736	5059	5135±89	4917±86	5129
Sc	5970±82	8924.04	5631.23	5564	5250	5449	5906±76	5850±71	5484
Ti	5395±97	9294.41	5856.49	5802	5704	5803	5873±63	5900±66	5809
V	6022±80	9605.22	6060.20	6040	6098	6121	6000±66	5936±67	6104
Cr	6155±45	9873.36	6242.34	6278	6432	6403	6479±55	6493±52	6369
Mn	6631±60	10107.40	6402.92	6516	6706	6649	6641±61	6498±54	6604
Fe	7116±58	10313.14	6541.94	6754	6920	6859	6726±37	6746±36	6809
Co	7038±56	10493.43	6659.39	6992	7074	7033	6991±51	7005±50	6984
Ni	7027±60	10651.78	6755.28	7230	7168	7171	7011±76	7011±72	7129
Cu	8425±17	10789.03	6829.62	7468	7202	7273	7994±96	8003±92	7244
Zn		10908.11	6882.39	7706	7176	7339			7329

TABLE 19. *Results for the parameter G_{ds}*

El.	Previous results	Hartree-Fock	DIAGON 1	DIAGON 2	DIAGON 3	DIAGON 4	ILS 3	Final ILS	Final GLS
Sc	1943±68	2007.15	1840.72	1574	1670	1637	1787±62	1930±65	1649
Ti	1719±56	1876.97	1728.73	1506	1625	1581	1538±37	1560±66	1590
V	1584±33	1795.01	1637.57	1470	1590	1541	1531±29	1563±30	1541
Cr	1590±19	1739.54	1567.26	1466	1565	1517	1513±24	1474±24	1514
Mn	1532±22	1700.66	1517.80	1494	1550	1509	1515±34	1501±37	1505
Fe	1536±24	1672.86	1489.17	1554	1545	1517	1561±19	1556±18	1514
Co	1607±33	1652.90	1481.39	1646	1550	1541	1554±46	1557±41	1541
Ni	1626±53	1638.76	1494.45	1770	1565	1581	1590±68	1589±65	1590
Cu	1550 (FIX)	1629.02	1528.35	1926	1590	1637	1274±86	1250±83	1649

TABLE 20. *Results for the parameter G**

El.	Previous results	Hartree-Fock	DIAGON 1	DIAGON 2	DIAGON 3	DIAGON 4	ILS 3	Final ILS	Final GLS
Sc	1943 (EQ.)	3223.33	2855.34	2282	2070	1868	2187±62	2161 (F.D.)	1880
Ti	1719 (EQ.)	2936.23	2689.36	2214	2025	1812	1938±37	1789 (F.D.)	1821
V	1584 (EQ.)	2751.21	2544.23	2178	1990	1772	2233±91	1794 (F.D.)	1772
Cr	1590 (EQ.)	2622.68	2419.94	2174	1965	1748	1784±87	1882±82	1745
Mn	1532 (EQ.)	2529.16	2316.48	2202	1950	1740	1915±34	1732 (F.D.)	1736
Fe	1536 (EQ.)	2458.99	2233.87	2262	1945	1748	1961±19	1787 (F.D.)	1745
Co	1607 (EQ.)	2405.28	2172.11	2354	1950	1772	1954±46	1788 (F.D.)	1772
Ni	1626 EQ.)	2363.57	2131.18	2478	1965	1812	1990±88	1820 (F.D.)	1821
Cu		2330.91	2111.11	2634	1990	1868	1674±101	1481 (F.D.)	1880

TABLE 21. *Results for the parameter H*

El.	Previous results	Hartree-Fock	DIAGON 1	DIAGON 2	DIAGON 3	DIAGON 4	ILS 3	Final ILS	Final GLS
Sc	275±18	323.61	313.20	158	238	224	331±27	310±31	215
Ti	175±7	267.45	267.36	144	197	204	184±5	184±4	192
V	150±6	224.55	226.76	130	162	184	165±6	166±5	169
Cr	157±4	190.00	191.38	116	133	164	166±5	161±5	146
Mn	70±6	161.19	161.23	102	110	144	100±8	121±9	123
Fe	85±6	136.54	136.31	88	93	124	92±5	90±5	100
Co	72±6	115.04	116.61	74	82	104	82±6	81±6	77
Ni	154±33	95.99	102.15	60	77	84	118±22	123±18	54

TABLE 22. *Results for the parameter H'*

El.	Previous results	Hartree-Fock	DIAGON 1	DIAGON 2	DIAGON 3	DIAGON 4	ILS 3	Final ILS	Final GLS
Ti	175 (EQ.)	189.71	199.65	104	141	144	141 (FIX)	124 (F.D.)	153
V	150 (EQ.)	152.87	159.04	90	106	124	35 ± 18	106 (F.D.)	130
Cr	157 (EQ.)	122.62	123.66	76	77	104	84 ± 15	61 ± 13	107
Mn	70 (EQ.)	97.00	93.51	62	54	84	54 (FIX)	61 (F.D.)	84
Fe	85 (EQ.)	74.76	68.59	48	37	64	37 (FIX)	30 (F.D.)	61
Co	72 (EQ.)	55.13	48.90	34	26	44	26 (FIX)	21 (F.D.)	38
Ni	154 (EQ.)	37.58	34.44	20	21	24	21 (FIX)	63 (F.D.)	15
Cu	0 (FIX)	21.65	25.20	6	22	4	22 (FIX)	4 (FIX)	0 (FIX)

TABLE 23. *Results for the parameter J*

El.	Previous results	Hartree-Fock	DIAGON 1	DIAGON 2	DIAGON 3	DIAGON 4	ILS 3	Final ILS	Final GLS
Ca	575 ± 20	2607.28	1485.69	1480	1260	1237	1260 (FIX)	1237 (FIX)	1112
Sc	1877 ± 96	2239.09	1367.98	1330	1040	1088	1668 ± 91	1579 ± 85	1066
Ti	1251 ± 53	2041.11	1263.71	1220	880	979	1326 ± 44	1313 ± 44	1036
V	972 ± 48	1907.24	1172.89	1150	780	910	992 ± 46	946 ± 40	1022
Cr	954 ± 32	1806.73	1095.51	1120	740	881	1061 ± 35	990 ± 31	1024
Mn	1294 ± 34	1726.42	1031.57	1130	760	892	1292 ± 56	1016 ± 55	1042
Fe	1183 ± 41	1659.47	981.08	1180	840	943	1004 ± 39	1025 ± 37	1076
Co	1245 ± 50	1601.79	944.02	1270	980	1034	1224 ± 55	1210 ± 55	1126
Ni	1144 ± 134	1550.86	920.42	1400	1180	1165	906 ± 89	913 ± 81	1192
Cu	(2446 ± 365)	1505.08	910.25	1570	1440	1336	1440 (FIX)	1336 (FIX)	1274

TABLE 24. *Results for the parameter J'*

El.	Previous results	Hartree-Fock	DIAGON 1	DIAGON 2	DIAGON 3	DIAGON 4	ILS 3	Final ILS	Final GLS
Sc	1877 (EQ.)	2250.32	1371.30	1610	1380	1540	2008 (F.D.)	2031 (F.D.)	1596
Ti	1251 (EQ.)	2134.09	1292.59	1500	1220	1431	1666 (F.D.)	1765 (F.D.)	1566
V	972 (EQ.)	2052.61	1227.31	1430	1120	1362	1675 (F.D.)	1337 ± 89	1552
Cr	954 (EQ.)	1990.63	1175.48	1400	1080	1333	1401 (F.D.)	1442 (F.D.)	1554
Mn	1294 (EQ.)	1940.85	1137.10	1410	1100	1344	1632 (F.D.)	1468 (F.D.)	1572
Fe	1183 (EQ.)	1899.24	1112.15	1460	1180	1395	1344 (F.D.)	1477 (F.D.)	1606
Co	1245 (EQ.)	1863.20	1100.65	1550	1320	1486	1564 (F.D.)	1662 (F.D.)	1656
Ni	1144 (EQ.)	1831.30	1102.59	1680	1520	1617	1246 (F.D.)	1365 (F.D.)	1722
Cu	(2446 (EQ.))	1802.11	1117.97	1850	1780	1788	1780 (FIX)	1788 (FIX)	1804
Zn		(1393.74)	1146.79	2060	2100	1999			1902

TABLE 25. *Results for the parameter K.*

El.	Previous results	Hartree-Fock	DIAGON 1	DIAGON 2	DIAGON 3	DIAGON 4	ILS 3	Final ILS	Final GLS
Ca	3795 ± 32	4824.07	3535.35	2710	2875	2930	2922 ± 98	2571 ± 83	3009
Sc	2551 ± 95	4001.34	3215.28	2515	2680	2741	2743 ± 85	2638 ± 82	2812
Ti	2415 ± 48	3590.97	2933.52	2370	2525	2586	2613 ± 30	2611 ± 29	2645
V	2468 ± 48	3324.70	2690.06	2275	2410	2465	2555 ± 42	2520 ± 39	2508
Cr	2311 ± 30	3130.26	2484.91	2230	2335	2378	2423 ± 33	2350 ± 29	2401
Mn	2599 ± 36	2977.82	2318.05	2235	2300	2325	2597 ± 46	2358 ± 52	2324
Fe	2459 ± 45	2852.49	2189.51	2290	2305	2306	2211 ± 51	2236 ± 36	2277
Co	2331 ± 55	2745.36	2099.27	2395	2350	2321	2328 ± 63	2323 ± 53	2260
Ni	2072 ± 135	2651.31	2047.34	2550	2435	2370	1980 ± 96	1982 ± 89	2273
Cu	(5090 ± 125)	2566.78	2033.70	2755	2560	2453	4122 ± 97	3864 ± 90	2316

TABLE 26. *Results for the parameter K'*

El.	Previous results	Hartree-Fock	DIAGON 1	DIAGON 2	DIAGON 3	DIAGON 4	ILS 3	Final ILS	Final GLS
Sc	3059 (F.D.)	3944.13	3670.74	3535	3480	3639	3543 (F.D.)	3536 (F.D.)	3759
Ti	2987 (F.D.)	3715.02	3427.99	3390	3325	3484	3413 (F.D.)	3509 (F.D.)	3592
V	3104 (F.D.)	3561.34	3229.81	3295	3210	3363	3342±73	2828±89	3455
Cr	3011 (F.D.)	3448.62	3076.21	3250	3135	3276	3353±88	3458±87	3348
Mn	3363 (F.D.)	3360.71	2967.18	3255	3100	3223	3397±74	3256 (F.D.)	3271
Fe	3287 (F.D.)	3288.84	2902.72	3310	3105	3204	3011±79	3134 (F.D.)	3224
Co	3223 (F.D.)	3227.54	2882.84	3415	3150	3219	3128±87	3221 (F.D.)	3207
Ni	3028 (F.D.)	3173.85	2907.54	3570	3235	3268	2780 (F.D.)	2880 (F.D.)	3220
Cu	(5090 (EQ.))	3124.84	2976.79	3775	3360	3351	4922 (F.D.)	4762 (F.D.)	3263
Zn		(2275.24)	3090.63	4030	3525	3468			3336

TABLE 27. *Results for the parameter ζ_d*

El.	Previous results	Hartree-Fock	DIAGON 1	DIAGON 2	DIAGON 3	DIAGON 4	ILS 3	Final ILS	Final GLS
Ca	18±9	27.94	47.87	10	1	0	1 (FIX)	0 (FIX)	0 (FIX)
Sc	58±21	59.25	60.81	80	49	41	53±26	34±28	13
Ti	114±29	97.59	90.04	150	103	90	99±25	97±24	73.5
V	141±22	145.93	135.56	220	163	147	148±34	172±33	139
Cr	247±24	206.17	197.37	290	229	212	235±26	238±25	209.5
Mn	321±28	280.14	275.46	360	301	285	215±41	228±41	285
Fe	410±23	369.69	369.85	430	379	366	367±38	341±23	365.5
Co	517±17	476.79	480.52	500	463	455	447±48	461±45	451
Ni	603±19	603.50	607.48	570	553	552	582±52	580±50	541.5

TABLE 28. *Results for the parameter ζ'_d*

El.	Previous results	Hartree-Fock	DIAGON 1	DIAGON 2	DIAGON 3	DIAGON 4	ILS 3	Final ILS	Final GLS
Sc	58 (EQ.)	79.12	80.69	100	35	42	78±42	79±35	15
Ti	114 (EQ.)	121.83	116.21	180	102	99	108±23	99±22	88.5
V	141 (EQ.)	174.62	168.01	260	175	164	149±19	160±20	167
Cr	247 (EQ.)	239.97	236.11	340	254	237	296±75	223±52	250.5
Mn	328 (EQ.)	319.65	320.49	420	339	318	368±51	343±55	339
Fe	410 (EQ.)	415.55	421.16	500	430	407	446±24	439±30	432.5
Co	517 (EQ.)	529.64	538.12	580	527	504	535±21	541±20	531
Ni	603 (EQ.)	663.96	671.37	660	630	609	639±22	640±22	634.5
Cu	836±3	820.74	820.91	740	739	722	860±48	847±42	743

TABLE 29. *Results for the parameter ζ''_d*

El.	Previous results	Hartree-Fock	DIAGON 1	DIAGON 2	DIAGON 3	DIAGON 4	ILS 3	Final ILS	Final GLS
Ti	114	146.57	142.38	210	101	108	117	101	103.5
V	141	205.25	200.46	300	187	181	150	148	195
Cr	247	275.91	274.85	390	279	262	357	208	291.5
Mn	328	361.53	365.52	480	377	351	521	458	393
Fe	410	464.00	472.48	570	481	448	525	537	499.5
Co	517	585.31	595.72	660	591	553	623	621	611
Ni	603	727.55	735.26	750	707	666	696	700	727.5
Cu	836 (EQ.)	892.91	891.09	840	829	787	950	912	849
Zn		1083.68	1063.20	930	957	916			975.5

TABLE 30. *Results for the parameter* ζ_p

El.	Previous results	Hartree-Fock	DIAGON 1	DIAGON 2	DIAGON 3	DIAGON 4	ILS 3	Final ILS	Final GLS
K			37.03	10	145	232			197
Ca	87±16	36.66	45.69	40	109	177	141±67	139±65	155
Sc	105±56	44.52	54.35	70	83	134	147±55	125±53	123
Ti	114±94	52.28	63.02	100	67	103	93±51	82±48	101
V	140±78	60.06	71.70	130	61	84	96±70	95±60	89
Cr	184±51	67.91	80.36	160	65	77	118±56	118±51	87
Mn	212±60	75.88	89.04	190	79	82	0 (FIX)	82 (FIX)	95
Fe	200±68	83.96	97.70	220	103	99	157±57	106±52	113
Co	236±53	92.14	106.38	250	137	128	111±58	187±54	141
Ni	255±51	100.38	115.05	280	181	169	263±71	270±71	179
Cu	375±8	108.71	123.71	310	235	222	208±94	201±82	227

TABLE 31. *Results for the parameter* ζ'_p

El.	Previous results	Hartree-Fock	DIAGON 1	DIAGON 2	DIAGON 3	DIAGON 4	ILS 3	Final ILS	Final GLS
Ca	89 (EQ.)	63.40	77.59	100	244	333	277 (F.D.)	295(F.D.)	294
Sc	105 (EQ.)	79.93	101.90	130	222	290	190±55	185±52	262
Ti	114 (EQ.)	96.20	126.22	160	210	259	176±59	192±57	240
V	140 (EQ.)	112.88	150.55	190	208	240	156±57	137±51	228
Cr	184 (EQ.)	130.15	174.86	220	216	223	230±49	268±40	226
Mn	212 (EQ.)	148.07	199.19	250	234	238	370±52	377±46	234
Fe	200 (EQ.)	166.68	223.50	280	262	255	339±56	278±52	252
Co	236 (EQ.)	185.90	247.82	310	300	284	270±62	246±61	280
Ni	255 (EQ.)	205.76	272.15	340	348	325	324±63	323±62	318
Cu	375 (EQ.)	226.17	296.46	370	406	378	408±74	388±68	366
Zn		247.11	320.79	400	474	443			424

TABLE 32. *Results for the parameter* ζ''_p

El.	Previous results	Hartree-Fock	DIAGON 1	DIAGON 2	DIAGON 3	DIAGON 4	ILS 3	Final ILS	Final GLS
Sc	105	131.98	149.95	190	361	446	333	245	401
Ti	114	157.90	189.42	220	353	415	259	302	379
V	140	185.31	229.40	250	355	396	216	179	367
Cr	184	214.35	269.36	280	367	389	342	418	365
Mn	212	245.08	309.34	310	389	394	740	772	373
Fe	200	277.51	349.30	340	421	411	521	450	391
Co	236	311.61	389.28	370	463	440	429	305	419
Ni	255	347.35	429.25	400	515	481	385	376	457
Cu	375	384.69	469.22	430	577	534	608	575	505
Zn		423.56	509.19	460	649	599			563
Ga		463.94	549.16	490	731	676			631

TABLE 33. *Results for the parameter* $\alpha = \alpha' = \alpha''$

El.	Previous results	DIAGON 1	DIAGON 2	DIAGON 3	DIAGON 4	ILS 3	Final ILS	Final GLS
Sc	50 (FIX)	60	23	31	28	54±9	28 (FIX)	19
Ti	43±4	60	29	33	30	19±6	18±5	22.5
V	54±2	60	35	35	32	37±6	24±5	26
Cr	63±1	60	41	37	34	37±6	32±4	29.5
Mn	73±2	60	47	39	36	16±6	15±5	33
Fe	74±2	60	53	41	38	40±3	39±3	36.5
Co	71±3	60	59	43	40	39±5	37±5	40
Ni	83±7	60	65	45	42	55±7	52±7	43.5
Cu		60	71	47	44		44 (FIX)	47

TABLE 34. *Results for the parameter* $\beta = \beta' = \beta''$

EL.	DIAGON 1	DIAGON 2	DIAGON 3	DIAGON 4	ILS 3	FINAL ILS	FINAL GLS
Sc	0	−250	−20	−308	−20 (FIX)	−308 (FIX)	−435
Ti	0	−250	−110	−350	−173±76	−243±69	−458
V	0	−250	−200	−392	−507±67	−740±68	−481
Cr	0	−250	−290	−434	−506±68	−426±62	−504
Mn	0	−250	−380	−476	−634±72	−637±68	−527
Fe	0	−250	−470	−518	−470 (FIX)	−518 (FIX)	−550
Co	0	−250	−560	−560	−560 (FIX)	−560 (FIX)	−573
Ni	0	−250	−650	−602	−650 (FIX)	−602 (FIX)	−596
Cu	0	−250	−740	−644	−740 (FIX)	−644 (FIX)	−619

TABLE 35. *Results for the parameter* $T = T' = T''$

EL.	DIAGON 1	DIAGON 2	DIAGON 3	DIAGON 4	ILS 3	FINAL ILS	FINAL GLS
Sc	0	−4.5	−1.9	−1.7	−1.9 (FIX)	−1.7 (FIX)	−2.7
Ti	0	−4.1	−2.2	−2.1	−2.7±0.8	−2.6±0.7	−2.9
V	0	−3.7	−2.5	−2.5	−1.9±0.6	−2.7±0.6	−3.1
Cr	0	−3.3	−2.8	−2.9	−2.6±0.6	−3.2±0.5	−3.3
Mn	0	−2.9	−3.1	−3.3	−5.6±0.9	−5.6±0.7	−3.5
Fe	0	−2.5	−3.4	−3.7	−3.3±0.4	−3.1±0.3	−3.7
Co	0	−2.1	−3.7	−4.1	−4.0±0.8	−4.3±0.6	−3.9
Ni	0	−1.7	−4.0	−4.5	−4 (FIX)	−4.5 (FIX)	−4.1
Cu	0	−1.3	−4.3	−4.9	−4.3 (FIX)	−4.9 (FIX)	−4.3

TABLE 36. *Results for the parameter* $T_x = T_x' = T_x''$

EL.	DIAGON 1	DIAGON 2	DIAGON 3	DIAGON 4	ILS 3	FINAL ILS	FINAL GLS
Sc	0	−1.8	−1.4	−2.8	−1.4 (FIX)	−1.4 (FIX)	−2.6
Ti	0	−2.1	−1.7	−2.8	−1.7 (FIX)	−2.8 (FIX)	−2.6
V	0	−2.4	−2.0	−2.8	−2.0 (FIX)	−2.8 (FIX)	−2.6
Cr	0	−2.7	−2.3	−2.8	−2.3 (FIX)	−4.0±0.8	−2.6
Mn	0	−3.0	−2.6	−2.8	−2.6 (FIX)	−2.8 (FIX)	−2.6
Fe	0	−3.3	−2.9	−2.8	−2.9 (FIX)	−2.8 (FIX)	−2.6
Co	0	−3.6	−3.2	−2.8	−3.2 (FIX)	−6.0±0.8	−2.6
Ni	0	−3.9	−3.5	−2.8	−3.5 (FIX)	−2.8 (FIX)	−2.6
Cu	0	−4.2	−3.8	−2.8	−3.8 (FIX)	−2.8 (FIX)	−2.6

TABLE 37. *Results for the parameter* $F_1 = F_1' = F_1''$

EL.	DIAGON 1	DIAGON 2	DIAGON 3	DIAGON 4	ILS 3	FINAL ILS	FINAL GLS
Ca	0	−10	−45	−6	−45 (FIX)	−6 (FIX)	−13
Sc	0	−10	−43	−6	−43 (FIX)	−46±3	−13
Ti	0	−10	−41	−6	−12±4	−11±4	−13
V	0	−10	−39	−6	−10±3	−13±4	−13
Cr	0	−10	−37	−6	−19±4	−6 (FIX)	−13
Mn	0	−10	−35	−6	−30±5	−14±4	−13
Fe	0	−10	−33	−6	−30±4	−30±3	−13
Co	0	−10	−31	−6	−19±6	−14±6	−13
Ni	0	−10	−29	−6	−42±6	−38±6	−13
Cu	0	−10	−27	−6	−27 (FIX)	−6 (FIX)	−13
Zn	0	−10	−25	−6			−13

TABLE 38. *Results for the parameter G_2*

EL.	DIAGON 1	DIAGON 2	DIAGON 3	DIAGON 4	ILS 3	FINAL ILS	FINAL GLS
Ca	0	1	0	13	0 (FIX)		9
Sc	0	5	0	13	27±9	14±4	9
Ti	0	9	0	13	0 (FIX)	0 (FIX)	9
V	0	13	0	13	21±6	11±3	9
Cr	0	17	0	13	0 (FIX)	4±3	9
Mn	0	21	0	13	24±9	3±3	9
Fe	0	25	0	13	30±6	28±4	9
Co	0	29	0	13	0 (FIX)	5±3	9
Ni	0	33	0	13	0 (FIX)	9±4	9

TABLE 39. *Results for the parameter G_2'*

EL.	DIAGON 1	DIAGON 2	DIAGON 3	DIAGON 4	ILS 3	FINAL ILS	FINAL GLS
Sc	0	5	15	13	27 (EQ.)	14 (EQ.)	9
Ti	0	9	15	13	15 (FIX)	0 (FIX)	9
V	0	13	15	13	21 (EQ.)	11 (EQ.)	9
Cr	0	17	15	13	15 (FIX)	4 (EQ.)	9
Mn	0	21	15	13	24 (EQ.)	3 (EQ.)	9
Fe	0	25	15	13	30 (EQ.)	28 (EQ.)	9
Co	0	29	15	13	15 (FIX)	5 (EQ.)	9
Ni	0	33	15	13	15 (FIX)	9 (EQ.)	9
Cu	0	37	15	13	15 (FIX)	13 (FIX)	9

TABLE 40. *Results for the parameter G_2''*

EL.	DIAGON 1	DIAGON 2	DIAGON 3	DIAGON 4	ILS 3	FINAL ILS	FINAL GLS
Ti	0	9	30	13	30 (FIX)	0 (FIX)	9
V	0	13	30	13	21	11	9
Cr	0	17	30	13	30 (FIX)	4	9
Mn	0	21	30	13	24	3	9
Fe	0	25	30	13	30	28	9
Co	0	29	30	13	30 (FIX)	5	9
Ni	0	33	30	13	30 (FIX)	9	9
Cu	0	37	30	13	30 (FIX)	13 (FIX)	9
Zn	0	41	30	13			9

TABLE 41. *Results for the mean error Δ in the ILS.*

EL.	Previous results	ILS 3	FINAL ILS
Ca	22.8	52.7	45.6
Sc	126.4	112.3	108.7
Ti	261.4	129.8	124.0
V	215.8	164.2	161.1
Cr	183.1	137.6	132.4
Mn	169.9	161.2	157.6
Fe	213.4	159.2	152.8
Co	164.2	146.3	140.2
Ni	131.1	112.5	106.3
Cu	12[a]	89.2[b]	82.8[b]

[a] Based on 18 levels.
[b] Based on 23 levels.

TABLE 42. *General interpolation parameters preliminary iterations*

PAR.	INITIAL	GLS 1	GLS 1a	GLS 2	GLS 2a	GLS 2b	GLS 3	GLS 3a	GLS 3b	GLS 3c
D_0'	1610.69	860±31	543±108	773±32	713±67	795±40	948±37	585±79	906±38	974±39
D_0''	28623.08	28482±62	26086±236	28746±81	28674±107	28350±92	28682±81	28723±101	28665±87	28527±*110*
D_1'	3892.39	3641±16	3550±42	3673±16	3614±22	3661±16	3688±16	3487±29	3703±18	3709±16
D_1''	5951.37	5719±21	5278±164	5711±20	5898±44	5738±27	5738±20	5832±80	5731±29	5740±30
D_2'	0	−123±4	−133±5	−128±5	−130±5	−123±5	−117±5	−135±9	−120±5	−115±5
D_2''	0	−123	−238±67	−128	−127±13	−123	−117	−94±12	−120	−115
B_0	769	734±8	745±13	727±6	734±6	731±5	717±5	735±8	712±6	719±5
B_0'	853	863±6	854±7	849±4	849±4	852±3	848±3	840±5	845±4	848±3
B_0''	937	992	963	971	964	973	979	945	978	977
B_1	67	52±2	57±3	53±2	57±2	55±2	52±2	60±3	52±2	52±2
B_1'	61	62±2	59±2	60±2	57±2	59±2	61±2	57±2	61±2	60±2
B_1''	55	72	61	67	57	63	70	54	70	68
C_0	2802	2898±31	2889±50	2954±30	2896±42	2935±25	2988±21	2919±42	2998±25	2988±26
C_0'	3133	3255±28	3258±49	3319±26	3325±22	3306±20	3338±19	3361±37	3340±19	3332±20
C_0''	3464	3612	3627	3684	3754	3677	3688	3803	3682	3676
C_1	244	408±8	402±14	433±7	419±13	429±8	437±8	413±11	429±9	438±9
C_1'	220	304±7	317±12	354±7	353±11	347±9	351±8	357±11	351±9	352±9
C_1''	196	200	232	275	287	265	265	301	273	266
$(G_3)_1$	−1.54	−7.0±2.0	0.1±2.2	2.2±0.7	1.8±1.1	0.3±0.5	0 (FIX)	−0.8±1.1	0.8±0.6	0 (FIX)
$(G_3')_1$	−0.97	−7.0±1.8	−2.2±2.0	2.2	−2.8±0.8	0.3	0	−3.5±1.2	0.8	0
$(G_3'')_1$	−0.40	−7.0	−4.3	2.2	−7.4	0.3	0	−6.2	0.8	0
$(G_3)_2$	0.44	1.4±2.0	−0.9±0.3	0 (FIX)	−1.2±0.3	1.4±0.2	0 (FIX)	−1.1±0.3	0 (FIX)	0 (FIX)
$(G_3')_2$	0.20	−1.4	−1.1±0.3	0	−1.0±0.3	−1.4	0	−1.1	0	0
$(G_3'')_2$	−0.04	−1.4	−1.3	0	−0.8	−1.4	0	−1.1	0	0
$(G_{ps})_0$	6295.11	6516±37	6451±76	6406±36	6517±42	6494±33	6469±33	6597±46	6443±34	6515±33
$(G_{ps})_1$	149.80	238±13	244±38	244±12	258±16	292±13	228±9	287±20	230±10	259±11
$(G_{ps})_2$	−10.78	−2±3	−24±5	−33±5	−24±5	−11±4	−18±4	−16±6	−19±4	−15±4
$(G_{ds})_0$	1622.01	1654±28	1626±45	1599±28	1647±30	1724±25	1589±22	1641±34	1580±23	1589±24
$(G^*)_0$	2420.66	2362 (F.D.)	3030±425	1985±76	2350±183	2432 (F.D.)	1664±68	4913±365	1707±72	1767±71
$(G_{ds})_1$	−39.05	44±8	24±27	−11±7	16±8	6.5±4.2	−10 (FIX)	13±8	−10±5	−5.5±3.3
$(G^*)_1$	−93.02	44	430±86	−11	148±83	179±45	−10	373±94	−10	−5.5
$(G_{ds})_2$	10.42	16±3	9.1±4.0	5.0±3.2	12±3	17±3	8.7±2.1	13.5±3.8	6.6±2.5	8.2±2.7
$(G^*)_2$	10.42	16	9	5.0	12	17	8.7	216±70	6.6	8.2
H_0	187.37	102±9	120±9	140±9	136±7	139±7	144±3	122±10	119±7	144±3
H_0'	119.65	68 (F.D.)	−117±47	106 (F.D.)	−54±21	105 (F.D.)	88 (F.D.)	43±54	84 (FIX)	51±12
H_1	−27.53	−14±5	−23±5	−20±2	−21±2	−22±2	−20±2	−21±2	−*22*±2	−20±2
H_1'	−27.53	−14	−78±11	−20	−48±9	−5.6±4.0	−20	−30±16	−22	−20
H_2	2.61	1.0±0.8	−0.7±0.8	3.2±1.1	1.8±0.9	3.0±0.9	3 (FIX)	−0.1±1.2	−0.2±1.0	3 (FIX)
H_2'	2.61	1.0	−0.7	3.2	1.8	3.0	3	10±6	−0.2	3
J_0	1098.80	1328±48	981±80	1058±47	1047±50	1076±47	1125±39	1021±68	1118±41	1063±42

TABLE 42. *General Interpolation Parameters Preliminary Iterations continued.*

PAR.	INITIAL	GLS 1	GLS 1a	GLS 2	GLS 2a	GLS 2b	GLS 3	GLS 3a	GLS 3b	GLS 3c
J_0'	1204.32	1612±67	832±307	1362±62	583±172	1356 (F.D.)	1702±60	784±229	1676±70	1687±72
J_1	−57.21	30±9	29±41	55±9	37±13	45±10	9.3±5.8	−11±18	6.4±5.1	−10±6
J_1'	−31.67	38±12	−322±70	55	−319±54	−46±21	9.3	−308±78	6.4	−10
J_2	6.72	20±5	4±5	59±9	7.6±5.6	6.7±5.1	5.5±3.2	5.2±7.0	5.1±4.7	0.6±4.9
J_2'	6.72	20	4	59	7.6	6.7	5.5	−53±29	5.1	0.6
K_0	2509.57	2485±53	2563±76	2497±50	2451±46	2412±35	2491±39	2336±73	2449±41	2437±42
K_0'	3190.04	3506±88	2788±213	3288±73	2839±110	3432 (F.D.)	3489±58	2696±190	3426±62	3525±61
K_1	−147.70	30±7	−46±37	−18±7	−44±13	−59±10	−57±10	−96±22	−53±11	−85±11
K_1'	−86.74	34±11	−185±98	−18	−138±36	39±14	−57	−193±75	−53	17±7
K_2	19.15	26±4	34±5	18±5	17±5	11±4	13±4	7.6±6.9	9.0±4.2	9.4±4.3
K_2'	22.29	26	−54±11	18	−31±9	11	13	−43±19	9.0	9.4
$(F_2)_0$	205.11	200±7	175±10	176±5	173±5	181±4	188±4	181±5	189±5	187±4
$(F_2')_0$	275.06	299±4	292.5±6	289±4	288±4	299±3	299±3	289±4	301±3	301±3
$(F_2'')_0$	345.01	398	410	402	403	417	410	397	413	415
$(F_2)_1$	−13.65	5.9±2.1	5.2±4.0	5.7±1.9	7.3±1.4	7.6±1.6	1.9±1.0	6.4±2.0	7.5±1.7	3.7±1.1
$(F_2')_1$	−7.68	4.1±1.5	2.9±3.1	2.3±1.4	−2.9±1.3	1.7±1.2	1.9	−3.4±2.1	−0.4±1.1	3.7
$(F_2'')_1$	−1.71	2.3	0.6	−1.1	−13.1	−4.2	1.9	−13.2	−8.3	3.7
$(F_2)_2 = (F_2')_2 =$										
$(F_2'')_2$	0	0 (FIX)	0±0.4	0 (FIX)	−2.1±1.6	0 (FIX)	0 (FIX)	0 (FIX)	0 (FIX)	0 (FIX)
$(G_1)_0$	254.21	205±7	241±9	225±4	237±5	229±4	233±4	233±6	229±4	230±4
$(G_1')_0$	267.65	254±5	265±7	259±3	271±4	261±4	260±3	259±4	258±3	262±3
$(G_1'')_0$	281.09	303	289	293	305	293	287	285	287	294
$(G_1)_1$	−25.98	−5±2	−17±5	−19±2	−15±2	−17±2	−19±1	−17±2	−16±1	−18±1
$(G_1')_1$	−15.07	−19±2	−16±5	−14±2	−16±2	−19±1	−19	−17±2	−16	−18
$(G_1'')_1$	−4.16	−33	−15	−9	−17	−21	−19	−17	−16	−18
$(G_1)_2$	7.83	0 (FIX)	2.5±0.6	0 (FIX)	1.8±0.6	1.1±0.4	0 (FIX)	0.9±0.3	0 (FIX)	0 (FIX)
$(G_1')_2$	3.54	0	0.6±0.7	0	1.2±0.5	1.1	0	0 (FIX)	0	0
$(G_1'')_2$	−0.75	0	−1.3	0	0.6	1.1	0	0	0	0
$(G_3)_0$	16.22	26±3	4.1±5.9	10±1	−2.0±3.2	2.5±1.7	15±2	1.9±3.1	13±2	14±2
$(G_3')_0$	18.96	32±3	11±3	10	11±3	2.5	23±1	11±3	24±2	24±1
$(G_3'')_0$	21.70	38±2	18	10	24	2.5	31	20	35	34
$(\zeta_d)_0$	356.97	360±39	337±45	331±26	352±24	339±21	322±24	354±31	326±26	332±25
$(\zeta_d')_0$	401.94	421±20	367±19	369±18	368±15	370±14	358±16	363±21	372±17	368±17
$(\zeta_d'')_0$	446.92	482	397	407	384	401	394	372	418	404
$(\zeta_d)_1$	86.24	70±12	73±26	78±10	81±8	76±8	84±8	87±11	82±9	85±9
$(\zeta_d')_1$	92.53	79±11	96±15	89±6	90±4	89±5	87±5	90±6	91±6	90±6
$(\zeta_d'')_1$	98.81	88	119	100	99	102	90	93	100	95
$(\zeta_d)_2$	8.14	2.3±1.8	2.2±3.1	2.7±1.6	6.9±2.9	2.8±1.9	3.7±1.4	8.5±4.0	4.8±2.4	4.9±2.4
$(\zeta_d')_2$	8.14	2.3	3.3±2.3	2.7	2.3±2.3	2.8	3.7	2.5±3.0	4.8	4.9

TABLE 42. *General Interpolation Parameters Preliminary Iterations continued.*

PAR.	INITIAL	GLS 1	GLS 1a	GLS 2	GLS 2a	GLS 2b	GLS 3	GLS 3a	GLS 3b	GLS 3c
$(\zeta_r'')_2$	8.14	2.3	4.4	2.7	−2.3	2.8	3.7	−3.5	4.8	4.9
$(\zeta_p)_0$	89.03	190 ± 61	127 ± 68	129 ± 49	123 ± 39	103 ± 38	142 ± 38	123 ± 51	137 ± 40	125 ± 41
$(\zeta_p')_0$	199.19	252 ± 39	281 ± 39	284 ± 38	273 ± 29	279 ± 30	298 ± 30	280 ± 38	298 ± 32	305 ± 32
$(\zeta_p'')_0$	309.34	314	435	439	423	455	454	437	459	485
$(\zeta_p)_1$	8.67	31 ± 11	37 ± 35	19 ± 10	20 ± 14	16 ± 9	11 ± 8	18 ± 16	9.5 ± 7.1	10 ± 7
$(\zeta_p')_1$	24.32	31	21 ± 20	23 ± 9	24 ± 11	23 ± 10	11	22 ± 14	19 ± 8	10
$(\zeta_p'')_1$	39.97	31	5	27	28	30	11	26	29	10
$(\zeta_p)_2$	0	*0* (FIX)	*8.3* ± 4.3	*5.0* ± 4.0	*5.0* ± 4.3	*3.2* ± 2.8	6.2 ± 2.7	7.2 ± 5.6	4.0 ± 2.6	4.6 ± 2.5
$(\zeta_p')_2$	0	0	3.9 ± 3.2	5.0	2.4 ± 3.2	3.2	6.2	4.0 ± 4.2	4.0	4.6
$(\zeta_p'')_2$	0	0	0	5.0	−0.2	3.2	6.2	0.8	4.0	4.6
α_0	60	47 ± 5	42 ± 10	39 ± 3	45 ± 6	42 ± 3	36 ± 3	40 ± 7	37 ± 3	37 ± 3
α_0'	60	47	48 ± 6	39	39 ± 3	42	36	35 ± 4	37	37
α_0''	60	47	54	39	33	42	36	30	37	37
α_1	0	7.6 ± 1.2	8.5 ± 2.0	1.3 ± 1.1	2.0 ± 1.9	1.2 ± 1.1	1.7 ± 1.1	4.4 ± 2.5	2.8 ± 1.0	1.1 ± 1.2
α_1'	0	7.6	5.8 ± 1.7	1.3	1.1 ± 1.6	1.2	1.7	1.4 ± 2.2	2.8	1.1
α_1''	0	7.6	3.1	1.3	0.2	1.2	1.7	−1.6	2.8	1.1
β_0	0	−253 ± 41	−247 ± 196	−381 ± 66	−299 ± 100	−321 ± 52	−476 ± 48	−280 ± 115	−476 ± 51	−460 ± 50
β_0'	0	−253	−301 ± 138	−381	−365 ± 57	−321	−476	−507 ± 73	−476	−460
β_0''	0	−253	−355	−381	−431	−321	−476	−734	−476	−460
$\beta_1 = \beta_1' = \beta_1''$	0	0 (FIX)	−28 ± 39	−122 ± 43	−121 ± 38	−115 ± 34	−42 ± 22	−24 ± 39	−21 ± 16	−53 ± 19
T_0	0	−2.9 ± 0.6	−2.2 ± 0.9	−3.1 ± 0.3	−2.3 ± 0.5	−2.7 ± 0.4	−3.3 ± 0.3	−3.2 ± 0.7	−3.2 ± 0.3	−3.3 ± 0.3
T_0'	0	−2.9	−1.7 ± 0.6	−3.1	−3.4 ± 0.3	−3.2 ± 0.3	−3.3	−3.5 ± 0.4	−3.2	−3.3
T_0''	0	−2.9	−1.2	−3.1	−4.5	−3.7	−3.3	−3.8	−3.2	−3.3
$T_1 = T_1' = T_1''$	0	0.4 ± 0.2	0.3 ± 0.2	−0.4 ± 0.2	−0.3 ± 0.2	−0.3 ± 0.2	−0.4 ± 0.2	−0.2 ± 0.2	−0.3 ± 0.2	−0.4 ± 0.2
$(T_r)_0$	0	−3.1 ± 0.9	−4.7 ± 1.2	−2.6 ± 0.6	−3.1 ± 0.8	−2.4 ± 0.5	−2.8 ± 0.6	−3.5 ± 1.0	−2.6 ± 0.6	−2.7 ± 0.6
$(T_r')_0$	*0*	−3.1	−3.2 ± 0.9	*−2.6*	−2.1 ± 0.6	−2.4	−2.8	−1.9 ± 0.7	*−2.6*	−2.7
$(T_r'')_0$	0	−3.1	−1.7	−2.6	−1.1	−2.4	−2.8	−0.3	−2.6	−2.7
$(T_r)_1 = (T_r')_1 = (T_r'')_1$	0	−0.3 ± 0.2	−0.3 ± 0.2	−0.3 ± 0.2	−0.3 ± 0.2	−0.3 ± 0.2	0 (FIX)	0.1 ± 0.3	0.1 ± 0.3	0 (FIX)
$(F_1)_0$	0	−12 ± 4	−40 ± 11	−35 ± 5	−38 ± 9	−18 ± 5	−6.2 ± 4.1	−28 ± 8	−8.1 ± 3.7	−7.0 ± 3.8
$(F_1')_0$	0	−12	−18 ± 3	−35	−33 ± 8	−18	−6.2	−27 ± 9	−8.1	−7.0
$(F_1'')_0$	0	−12	4	−35	−28	−18	−6.2	−26	−8.1	−7.0
$(F_1)_1$	0	0 (FIX)	2.8 ± 3.8	2.6 ± 1.9	7.8 ± 4.2	3.1 ± 2.3	2 (FIX)	−1.6 ± 2.8	−5.0 ± 1.6	−3.9 ± 2.0
$(F_1')_1$	0	0	−7.6 ± 2.6	2.6	−9.1 ± 2.8	3.1	2	−12 ± 4	−5.0	−3.9
$(F_1'')_1$	0	0	−18	2.6	−26	3.1	2	−22	−5.0	−3.9
$(G_1)_0$	0	21 ± 5	−4.2 ± 10	−6.6 ± 5.1	−7.4 ± 5.3	2.8 ± 4.0	13 ± 3	−5.4 ± 6.9	3.2 ± 3.0	5.9 ± 3.1
$(G_1')_0$	0	21	29 ± 9	−6.6	25.2 ± 4.8	23 ± 4	13	19 ± 6	3.2	5.9
$(G_1'')_0$	*0*	21	*62*	*−6.6*	*57.8*	43	13	43	2.3	5.9
$(G_1)_1$	0	4.7 ± 1.2	−0.2 ± 2.1	0.8 ± 1.1	4.3 ± 2.2	2.0 ± 1.6	0 (FIX)	−0.4 ± 1.7	1.3 ± 1.1	0 (FIX)
$(G_1')_1$	0	4.7	6.0 ± 2.0	0.8	−0.1 ± 2.2	2.0	0	−1.9 ± 1.8	1.3	0
$(G_1'')_1$	0	4.7	12	0.8	−4.5	2.0	0	−3.4	1.3	0

TABLE 42. *General Interpolation Parameters Preliminary Iterations continued.*

PAR.	INITIAL	GLS 1	GLS 1a	GLS 2	GLS 2a	GLS 2b	GLS 3	GLS 3a	GLS 3b	GLS 3c
M_0	13020	13030 ± 159	13049 ± 170	13051 ± 180	13048 ± 179	13037 ± 161	13073 ± 126	13065 ± 172	13060 ± 131	13061 ± 131
M_1	35800	37641 ± 96	37643 ± 119	37840 ± 98	37580 ± 127	37600 ± 89	37651 ± 88	37700 ± 174	37682 ± 94	37655 ± 95
M_2	35070	35281 ± 86	35278 ± 109	35332 ± 86	35252 ± 120	35298 ± 80	35333 ± 83	35304 ± 96	35339 ± 87	35344 ± 86
M_3	38690	38515 ± 84	38486 ± 108	38552 ± 84	38504 ± 116	38571 ± 80	38521 ± 82	38467 ± 96	38514 ± 84	38545 ± 85
M_4	43540	43757 ± 88	43807 ± 102	43798 ± 82	43796 ± 110	43863 ± 80	43724 ± 83	43721 ± 98	43722 ± 87	43748 ± 86
M_5	59160	58916 ± 83	59013 ± 90	58888 ± 79	58911 ± 100	58978 ± 77	58794 ± 78	58878 ± 96	58798 ± 86	58820 ± 84
M_6	70910	67536 ± 78	67669 ± 77	67465 ± 72	67504 ± 87	67551 ± 71	67382 ± 70	67607 ± 92	67390 ± 75	67400 ± 68
M_7	51750	51974 ± 67	52177 ± 61	51869 ± 74	51934 ± 69	51930 ± 60	51779 ± 58	51936 ± 79	51792 ± 67	51786 ± 65
M_8	42130	42285 ± 51	42548 ± 42	42158 ± 54	42230 ± 47	42183 ± 43	42071 ± 47	42481 ± 69	42085 ± 48	42065 ± 49
M_9	31370	31914 ± 73	32269 ± 103	31784 ± 88	31865 ± 113	31766 ± 67	31639 ± 71	31970 ± 102	31642 ± 74	31618 ± 75
M_{10}	30700	32238 ± 75	32681 ± 65	32118 ± 84	32189 ± 71	32039 ± 68	31857 ± 70	32227 ± 91	31846 ± 78	31812 ± 77
M''_{11}	94502	92090 ± 183	91674 ± 310	92033 ± 191	92430 ± 239	91861 ± 164	92261 ± 120	92580 ± 118	92142 ± 128	92166 ± 127
M''_{12}	551	570 ± 160	527 ± 173	597 ± 180	561 ± 181	594 ± 162	583 ± 108	566 ± 171	598 ± 116	591 ± 119
Δ		205.0	193.9	200.3	188.2	203.1	196.7	187.8	198.1	194.5

TABLE 43. *General Interpolation Parameters Final Iteration*

PAR.	GLS 4	GLS 4a	GLS 4b	GLS 4c	GLS 4d	GLS 4e	GLS 4f	GLS 4g	GLS 4h	GLS 4i
D_0'	963 ± 31	612 ± 105	920 ± 36	895 ± 38	929 ± 36	965 ± 32	968 ± 33	1007 ± 34	1039 ± 35	1041 ±;37
D_0''	28770 ± 72	28599 ± 98	28689 ± 82	28745 ± 81	28683 ± 74	2873 ± 77	28739 ± 78	28784 ± 77	28704 ± 79	28703 ± 83
D_1'	3701 ± 15	3592 ± 46	3691 ± 17	3690 ± 17	3699 ± 17	3706 ± 17	3706 ± 16	3723 ± 17	3720 ± 19	3724 ± 19
D_1''	5784 ± 32	5818 ± 58	5736 ± 35	5754 ± 32	5748 ± 31	5791 ± 33	5794 ± 32	5814 ± 31	5813 ± 33	5822 ± 35
D_2'	−114 ± 4	−126 ± 10	−116 ± 5	−114 ± 5	−116 ± 5	−115 ± 5	−117 ± 5	±120 ± 5	−120 ± 6	−121 ± 6
D_2''	−114	−100 ± 15	−116	−114	−116	−115	−117	−120	−120	−121
B_0	714 ± 4	727 ± 7	714 ± 5	716 ± 5	714 ± 5	712 ± 5	700 ± 4	705 ± 4	714 ± 4	712 ± 4
B_0'	844 ± 3	839 ± 4	842 ± 3	841 ± 3	842 ± 3	844 ± 3	839 ± 3	843 ± 3	855 ± 3	855 ± 3
B_0''	974	951	970	966	970	976	978	981	996	998
B_1	51 ± 2	57 ± 3	51 ± 2	51 ± 2	51 ± 2	51 ± 2	45 ± 2	51 ± 2	52 ± 2	52 ± 2
B_1'	60 ± 1	57 ± 2	60 ± 2	58 ± 2	59 ± 2	61 ± 2	55 ± 2	63 ± 1	63 ± 1	63 ± 1
B_1''	69	57	69	65	67	71	65	75	74	74
C_0	3013 ± 19	2938 ± 46	3005 ± 27	3010 ± 26	3005 ± 22	3016 ± 22	3099 ± 20	2916 ± 15	2839 ± 15	2843 ± 13
C_0'	3362 ± 16	3376 ± 26	3359 ± 23	3364 ± 23	3359 ± 21	3361 ± 18	3433 ± 17	3267 ± 12	3190 ± 10	3191 ± 9
C_0''	3711	3814	3713	3718	3713	3706	3767	3618	3541	3539
C_1	433 ± 7	426 ± 15	441 ± 11	448 ± 11	440 ± 8	437 ± 8	450 ± 8	413 ± 7	412 ± 7	414 ± 8
C_1'	348 ± 7	362 ± 13	358 ± 10	362 ± 10	358 ± 8	350 ± 8	362 ± 8	322 ± 7	319 ± 6	320 ± 6
C_1''	263	298	275	276	276	263	274	231	226	226
$(F_1)_0$	183 ± 3	190 ± 5	187 ± 4	186 ± 4	186 ± 4	180 ± 4	179 ± 4	180 ± 4	181 ± 5	178 ± 4
$(F_1')_0$	299 ± 3	293 ± 4	298 ± 3	290 ± 3	298 ± 3	299 ± 3	298 ± 3	298 ± 3	297 ± 4	297 ± 3
$(F_1'')_0$	415	396	410	394	410	418	417	416	413	416
$(F_2)_1$	2.5 ± 1.1	7.7 ± 1.8	2.5 ± 1	2.0 ± 1.0	2.1 ± 1.1	2.3 ± 1.1	2.2 ± 1.1	2.3 ± 1.1	2.5 ± 1.2	2.4 ± 1.2
$(F_2')_1$	2.5	−2.2 ± 2.0	2.5	2.0	2.1	2.3	2.2	2.3	2.5	2.4
$(F''_2)_1$	2.5	−12.1	2.5	2.0	2.1	2.3	2.2	2.3	2.5	2.4
$(F_2)_2 = (F_1')_2 =$										
$(F_2'')_2$	0 (FIX)	0 (FIX)	0 (FIX)	0 (FIX)	0 (FIX)	0 (FIX)	0 (FIX)	0 (FIX)	0 (FIX)	0 (FIX)
$(G_1)_0$	235 ± 3	236 ± 5	233 ± 4	237 ± 4	234 ± 4	228 ± 4	229 ± 4	230 ± 4	237 ± 4	231 ± 4
$(G_1')_0$	261 ± 3	260 ± 4	251 ± 3	259 ± 3	261 ± 3	256 ± 3	256 ± 3	256 ± 3	260 ± 3	256 ± 3
$(G_1'')_0$	287	284	269	281	288	284	283	282	283	281
$(G_1)_1$	−19 ± 1	−17 ± 2	−19 ± 1	−18 ± 1	−17 ± 1	−19 ± 1	−18 ± 1	−18 ± 1	−19 ± 1	−19 ± 1
$(G_1')_1$	−19	−18 ± 2	−19	−18	−17	−19	−18	−18	−19	−19
$(G_1'')_1$	−19	−19	−19	−18	−17	−19	−18	−18	−19	−19
$(G_1)_2$	0 (FIX)	0.7 ± 0.3	0 (FIX)	0 (FIX)	0 (FIX)	0 (FIX)	0 (FIX)	0 (FIX)	0 (FIX)	0 (FIX)
$(G_1')_2$	0	0.7	0	0	0	0	0	0	0	0
$(G_1'')_2$	0	0.7	0	0	0	0	0	0	0	0
$(G_3)_0$	13 ± 1	4.6 ± 2.8	14 ± 2	14 ± 1	14 ± 1	13 ± 1	13 ± 1	13 ± 1	14 ± 2	14 ± 1
$(G_3')_0$	21 ± 1	11.1 ± 2.6	22 ± 1	19 ± 2	22 ± 1	22 ± 1	22 ± 1	22 ± 1	20 ± 2	21 ± 1
$(G_3'')_0$	29	17.6	30	24	30	31	31	31	26	28
$(G_3)_1$	0 (FIX)	−0.5 ± 1.0	0 (FIX)	0 (FIX)	0 (FIX)	0 (FIX)	0 (FIX)	0 (FIX)	0 (FIX)	0 (FIX)
$(G_3')_1$	0	−3.5 ± 1.1	0	0	0	0	0	0	0	0

TABLE 43. *General Interpolation Parameters Final Iteration—continued*

PAR.	GLS 4	GLS 4a	GLS 4b	GLS 4c	GLS 4d	GLS 4e	GLS 4f	GLS 4g	GLS 4h	GLS 4i
$(G_3'')_1$	0	−6.5	0	0	0	0	0	0	0	0
$(G_3)_2$	0 (FIX)	−1.1 ±0.2	0 (FIX)	0 (FIX)	0 (FIX)	0 (FIX)	0 (FIX)	0 (FIX)	0 (FIX)	0 (FIX)
$(G_3')_2$	0	−1.1	0	0	0	0	0	0	0	0
$(G_3'')_2$	0	−1.1	0	0	0	0	0	0	0	0
$(G_{\rho\omega})_0$	6454 ±20	6601 ±49	6447 ±34	6555 ±37	6445 ±23	6446 ±23	6463 ±22	6462 ±23	6458 ±24	6469 ±26
$(G_{\rho\omega})_1$	220 ±10	257 ±18	222 ±10	280 ±13	221 ±10	222 ±10	221 ±10	219 ±11	217 ±11	219 ±11
$(G_{\rho\omega})_2$	−15 ±3	−4.6 ±5.6	−14 ±4	−10 ±4	−15 ±4	−17 ±4	−17 ±4	−19 ±4	−14 ±4	−16 ±4
$(G_{\omega\omega})_0$	1595 ±14	1660 ±30	1593 ±26	1587 ±25	1592 ±15	1579 ±17	1583 ±15	1584 ±15	1616 ±16	1601 ±18
$(G'')_0$	1826 (F.D.)	3107 ±801	1649 ±83	1674 ±81	1829 (F.D.)	1810 (F.D.)	1814 (F.D.)	1815 (F.D.)	1847 (F.D.)	1832 (F.D.)
$(G_{\omega\omega})_1$	0 (FIX)	14 ±9	0 (FIX)	0 (FIX)	0 (FIX)	0 (FIX)	0 (FIX)	0 (FIX)	0 (FIX)	0 (FIX)
$(G'')_1$	0	544 ±241	0	0	0	0	0	0	0	0
$(G_{\omega\omega})_2$	8.7 ±1.2	15 ±3	8.1 ±2.9	6.8 ±2.6	8.1 ±1.9	9.0 ±1.7	9.0 ±1.6	8.7 ±1.8	9.0 ±1.7	9.2 ±1.8
$(G'')_2$	8.7	82 ±62	8.1	6.8	8.1	9.0	9.0	8.7	9.0	9.2
H_0	123 ±2	114 ±8	123 ±3	124 ±3	123 ±2	124 ±3	124 ±3	122 ±3	123 ±3	124 ±3
H_0'	84 (FIX)	88 ±47	84 (FIX)	42 ±15	84 (FIX)	84 (FIX)	84 (FIX)	84 (FIX)	84 (FIX)	84 (FIX)
H_1	−23 ±1	−24 ±2	−22 ±1	−23 ±1	−22 ±1	−23 ±1	−24 ±1	−24 ±1	−24 ±1	−24 ±2
H_1'	−23	−11 ±14	−22	−23	−22	−23	−24	−24	−24	−24
H_2	0 (FIX)	−1.3 ±1.1	0 (FIX)	0 (FIX)	0 (FIX)	0 (FIX)	0 (FIX)	0 (FIX)	0 (FIX)	0 (FIX)
H_2'	0	9.0 ±5.0	0	0	0	0	0	0	0	0
J_0	1122 ±21	1090 ±61	1134 ±47	1039 ±41	1123 ±25	1126 ±25	1127 ±24	1118 ±23	1126 ±24	1129 ±26
J_0'	1652 ±38	598 ±271	1693 ±70	975 ±74	1666 ±39	1695 ±36	1708 ±37	1685 ±40	1645 ±42	1689 ±43
J_1	26 ±3	−15 ±17	14 ±9	−2.8 ±1.9	19 ±6	11 ±6	15 ±5	−1.8 ±5.2	7.0 ±5.3	6.7 ±5.2
J_1'	26	−376 ±127	14	−231 ±37	19	11	15	−1.8	7.0	6.7
J_2	8.4 ±2.1	8.2 ±6.2	7.2 ±5	−1.4 ±3.1	6.1 ±3.0	6.9 ±3.2	7.5 ±3.1	5.0 ±3.2	8.1 ±3.1	6.6 ±4.2
J_2'	8.4	−32 ±27	7.2	−1.4	6.1	6.9	7.5	5.0	8.1	6.6
K_0	2474 ±29	2404 ±66	2508 ±36	2468 ±40	2485 ±28	2468 ±29	2467 ±28	2445 ±29	2476 ±30	2470 ±31
K_0'	3421 ±38	2984 ±209	3446 ±46	3182 ±51	3426 ±34	3463 ±38	3467 ±39	3435 ±37	3426 ±39	3467 ±41
K_1	−62 ±6	−93 ±20	−54 ±13	−76 ±13	−60 ±7	−61 ±8	−61 ±7	−67 ±7	−63 ±8	−62 ±9
K_1'	−62	−167 ±70	−54	−76	−60	−61	−61	−67	−63	−62
K_2	15 ±3	12 ±6	17 ±5	14 ±5	14 ±3	12 ±4	13 ±4	7.9 ±4.1	15 ±5	12 ±5
K_2'	15	−5.6 ±19	17	14	14	12	13	7.9	15	12
$(\zeta_a)_0$	310 ±19	343 ±28	319 ±25	327 ±24	323 ±18	311 ±17	308 ±18	315 ±19	314 ±20	315 ±21
$(\zeta_a')_0$	364 ±16	360 ±19	355 ±17	367 ±17	359 ±14	365 ±15	367 ±16	365 ±17	366 ±16	366 ±19
$(\zeta_a'')_0$	418	377	391	407	395	419	426	415	418	417
$(\zeta_a)_1$	78 ±5	82 ±10	82 ±9	84 ±9	82 ±6	77 ±7	77 ±8	78 ±8	77 ±9	76 ±10
$(\zeta_a')_1$	91 ±4	90 ±5	87 ±6	89 ±5	87 ±5	90 ±6	91 ±6	92 ±6	92 ±6	91 ±6
$(\zeta_a'')_1$	104	98	92	94	92	103	105	106	107	106
$(\zeta_a)_2$	2.6 ±1.2	5.5 ±3.5	1.9 ±1.6	3.2 ±2.1	2.4 ±1.5	2.5 ±1.8	2.3 ±1.7	3.0 ±1.5	2.8 ±1.6	2.7 ±1.4
$(\zeta_a')_2$	2.6	1.8 ±2.8	1.9	3.2	2.4	2.5	2.3	3.0	2.8	2.7
$(\zeta_a'')_2$	2.6	−1.9	1.9	3.2	2.4	2.5	2.3	3.0	2.8	2.7

TABLE 43. *General Interpolation Parameters Final Iteration—continued*

PAR.	GLS 4	GLS 4a	GLS 4b	GLS 4c	GLS 4d	GLS 4e	GLS 4f	GLS 4g	GLS 4h	GLS 4i
$(\zeta_p)_0$	143 ± 26	139 ± 46	149 ± 43	135 ± 42	150 ± 26	137 ± 28	140 ± 25	135 ± 27	130 ± 29	123 ± 30
$(\zeta_p')_0$	284 ± 19	278 ± 34	290 ± 34	279 ± 33	290 ± 19	269 ± 24	269 ± 21	269 ± 22	279 ± 25	264 ± 27
$(\zeta_p'')_0$	425	417	431	423	430	401	398	403	428	405
$(\zeta_p)_1$	13 ± 5	17 ± 17	15 ± 8	13 ± 8	18 ± 6	14 ± 6	15 ± 5	16 ± 6	15 ± 7	16 ± 7
$(\zeta_p')_1$	13	19 ± 13	15	13	18	14	15	16	15	16
$(\zeta_p'')_1$	13	21	15	13	18	14	15	16	15	16
$(\zeta_p)_2$	5.2 ± 1.7	5.4 ± 5.0	5.6 ± 3.2	5.3 ± 3.0	5.6 ± 1.9	5.3 ± 2.1	5.5 ± 2.0	5.4 ± 1.9	5.4 ± 2.0	5.5 ± 2.1
$(\zeta_p')_2$	5.2	3.6 ± 3.8	5.6	5.3	5.6	5.3	5.5	5.4	5.4	5.5
$(\zeta_p'')_2$	5.2	1.8	5.6	5.3	5.6	5.3	5.5	5.4	5.4	5.5
α_0	33 ± 2	42 ± 6	34 ± 3	33 ± 3	34 ± 3	34 ± 3	30 ± 3	61 ± 2	71 ± 1	72 ± 1
α_0'	33	32 ± 3	34	33	34	34	30	61	71	72
α_0''	33	22	34	33	34	34	30	61	71	72
α_1	3.7 ± 0.9	3.0 ± 2.3	1.6 ± 1.2	0.7 ± 1.1	1.5 ± 1.2	3.1 ± 1.1	2.9 ± 1.2	6.8 ± 1.1	7.1 ± 0.8	6.9 ± 0.7
α_1'	3.7	0.8 ± 2.0	1.6	0.7	1.5	3.1	2.9	6.8	7.1	6.9
α_1''	3.7	−1.4	1.6	0.7	1.5	3.1	2.9	6.8	7.1	6.9
β_0	−527 ± 28	−380 ± 102	−523 ± 37	−534 ± 38	−526 ± 31	−521 ± 30	−673 ± 31	−336 ± 32	0 (FIX)	0 (FIX)
β_0'	−527	−549 ± 65	−523	−534	−526	−521	−673	−336	0	0
β_0''	−527	−718	−523	−534	−526	−521	−673	−336	0	0
$\beta_1=\beta_1'=\beta_1''$	−23 ± 11	−59 ± 44	−65 ± 29	−89 ± 31	−40 ± 13	−22 ± 12	−51 ± 18	−7.2 ± 8.1	0 (FIX)	0 (FIX)
T_0	−3.5 ± 0.3	−2.6 ± 0.7	−3.4 ± 0.3	−3.5 ± 0.3	−3.4 ± 0.3	−3.5 ± 0.3	−3.8 ± 0.3	0 (FIX)	0 (FIX)	0 (FIX)
T_0'	−3.5	−3.7 ± 0.4	−3.4	−3.5	−3.4	−3.5	−3.8	0	0	0
T_0''	−3.5	−4.8	−3.4	−3.5	−3.4	−3.5	−3.8	0	0	0
$T_1=T_1'=T_1''$	−0.2 ± 0.1	−0.3 ± 0.2	−0.4 ± 0.2	−0.4 ± 0.2	−0.4 ± 0.2	−0.3 ± 0.2	−0.3 ± 0.2	0 (FIX)	0 (FIX)	0 (FIX)
$(T_s)_0$	−2.6 ± 0.6	−3.1 ± 0.9	−2.6 ± 0.6	−2.5 ± 0.5	−2.6 ± 0.5	−2.7 ± 0.6	0 (FIX)	0 (FIX)	0 (FIX)	0 (FIX)
$(T_s')_0$	−2.6	−2.0 ± 0.6	−2.6	−2.5	−2.6	−2.7	0	0	0	0
$(T_s'')_0$	−2.6	−0.9	−2.6	−2.5	−2.6	−2.7	0	0	0	0
$(T_s)_1=$ $(T_s')_1=(T_s'')_1$	0 (FIX)	0.1 ± 0.3	0 (FIX)	0 (FIX)	0 (FIX)	0 (FIX)	0 (FIX)	0 (FIX)	0 (FIX)	0 (FIX)
$(F_1)_0$	−13 ± 3	−14 ± 9	−8.6 ± 4.1	−21 ± 5	−11 ± 4	0 (FIX)	0 (FIX)	0 (FIX)	−13 ± 5	0 (FIX)
$(F_1')_0$	−13	−26 ± 9	−8.6	−21	−11	0	0	0	−13	0
$(F_1'')_0$	−13	−38	−8.6	−21	−11	0	0	0	−13	0
$(F_1)_1$	0 (FIX)	−1.9 ± 4.3	0 (FIX)	−4.0 ± 2.1	0 (FIX)	0 (FIX)	0 (FIX)	0 (FIX)	0 (FIX)	0 (FIX)
$(F_1')_1$	0	−11 ± 4	0	−4.0	0	0	0	0	0	0
$(F_1'')_1$	0	−20	0	−4.0	0	0	0	0	0	0
$(G_2)_0$	9 ± 3	4.2 ± 4.0	12 ± 3	10 ± 3	12 ± 3	0 (FIX)	0 (FIX)	0 (FIX)	9 ± 4	0 (FIX)
$(G_2')_0$	9	19 ± 4	12	10	12	0	0	0	9	0
$(G_2'')_0$	9	34	12	10	12	0	0	0	9	0
$(G_2)_1$	0 (FIX)	0.6 ± 2.4	0 (FIX)	0 (FIX)	0 (FIX)	0 (FIX)	0 (FIX)	0 (FIX)	0 (FIX)	0 (FIX)
$(G_2')_1$	0	−2.0 ± 2.9	0	0	0	0	0	0	0	0
$(G_2'')_1$	0	−4.6	0	0	0	0	0	0	0	0

TABLE 43. *General Interpolation Parameters Final Iteration—continued*

PAR.	GLS 4	GLS 4a	GLS 4b	GLS 4c	GLS 4d	GLS 4e	GLS 4f	GLS 4g	GLS 4h	GLS 4i
M_0	13065 ± 99	13057 ± 156	13066 ± 113	13062 ± 109	13060 ± 101	13062 ± 103	13061 ± 101	13060 ± 102	13059 ± 107	13057 ± 106
M_1	37650 ± 69	37629 ± 161	37646 ± 79	37644 ± 80	31647 ± 66	37652 ± 68	37658 ± 66	37681 ± 68	37678 ± 71	37681 ± 72
M_2	35331 ± 72	35300 ± 151	35337 ± 81	35332 ± 76	35339 ± 71	35332 ± 72	35343 ± 71	35356 ± 73	35365 ± 76	39230 ± 75
M_3	38522 ± 70	38524 ± 136	38533 ± 80	38539 ± 79	38533 ± 69	38524 ± 68	38544 ± 69	38538 ± 70	38566 ± 73	38569 ± 74
M_4	43725 ± 71	43773 ± 105	43738 ± 80	43750 ± 76	43732 ± 70	43722 ± 72	43742 ± 71	43719 ± 73	43771 ± 75	43770 ± 76
M_5	58792 ± 59	58887 ± 126	58808 ± 75	58819 ± 72	58798 ± 58	58789 ± 64	58786 ± 63	58764 ± 62	58837 ± 63	58836 ± 63
M_6	67352 ± 54	67506 ± 98	67367 ± 69	67364 ± 68	67355 ± 56	67347 ± 57	67330 ± 56	67302 ± 57	67379 ± 56	67374 ± 55
M_7	51757 ± 49	52013 ± 91	51772 ± 67	51761 ± 61	51756 ± 51	51754 ± 52	51720 ± 51	51701 ± 52	51789 ± 52	51783 ± 53
M_8	42032 ± 47	42398 ± 88	42063 ± 50	42042 ± 48	42042 ± 42	42027 ± 48	41994 ± 49	41961 ± 47	42016 ± 48	42008 ± 48
M_9	31585 ± 55	32095 ± 102	31644 ± 78	31619 ± 74	31614 ± 56	31580 ± 59	31558 ± 60	31493 ± 59	31511 ± 61	31504 ± 61
M_{10}	31759 ± 59	32429 ± 91	31868 ± 79	31829 ± 76	31823 ± 60	31752 ± 62	31758 ± 63	31652 ± 61	31653 ± 63	31646 ± 64
M''_{11}	92641 ± 94	92492 ± 146	92289 ± 103	92306 ± 102	93322 ± 96	92668 ± 102	92631 ± 101	92697 ± 103	92640 ± 101	92664 ± 99
M''_{12}	572 ± 102	559 ± 153	579 ± 105	573 ± 103	583 ± 101	569 ± 104	571 ± 103	573 ± 102	577 ± 104	574 ± 102
Δ	182.2	171.3	180.2	176.1	199.7	183.5	189.1	203.7	210.8	211.4

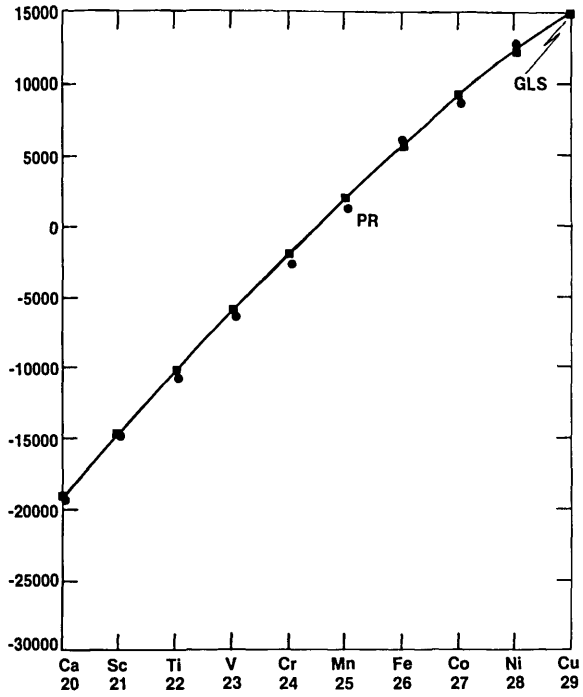

FIGURE 1. Plots of D' versus atomic number.

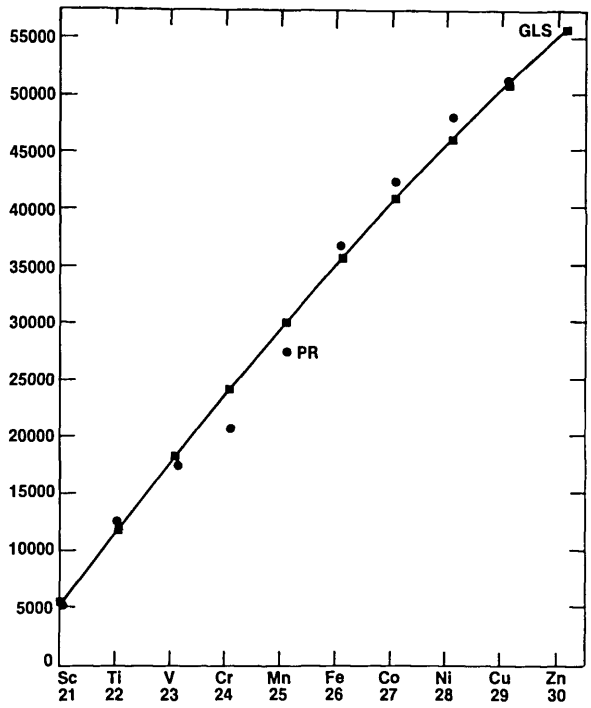

FIGURE 2. Plots of D'' versus atomic number.

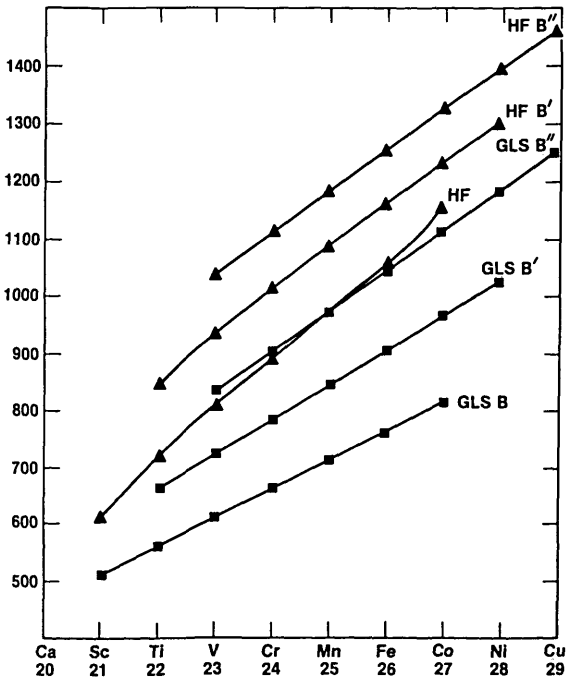

FIGURE 3. Plots of B, B', and B'' versus atomic number.

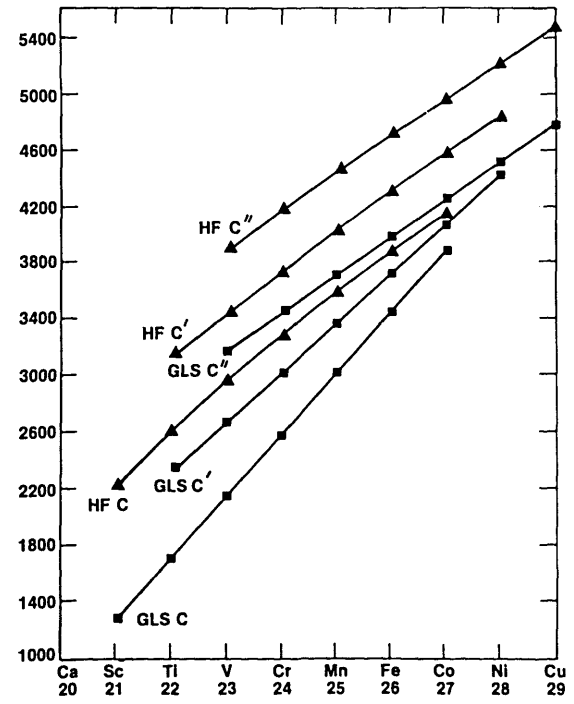

FIGURE 4. Plots of C, C', and C'' versus atomic number.

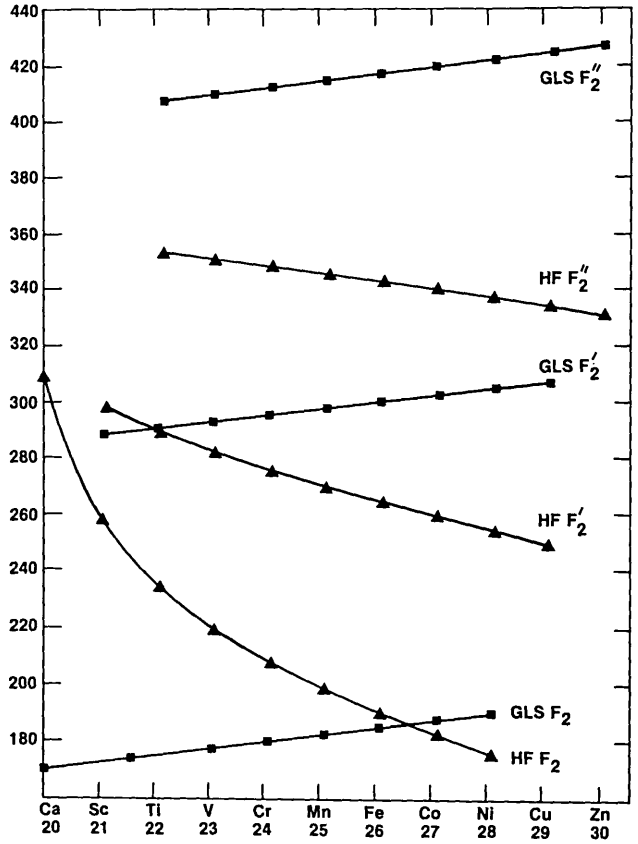

FIGURE 5. Plots of F_2, F_2', and F_2'' versus atomic number.

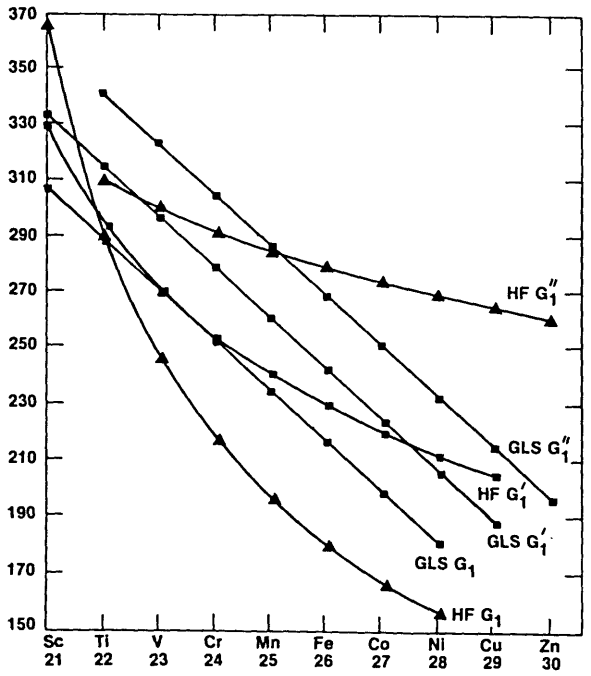

FIGURE 6. Plots of G_1, G_1', and G_1'' versus atomic number.

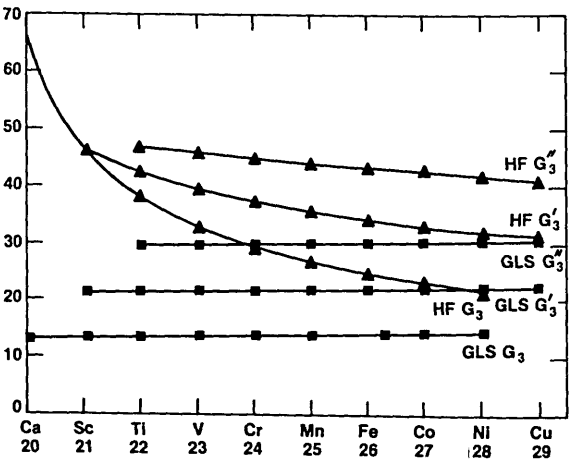

FIGURE 7. Plots of G_3, G_3', and G_3'' versus atomic number.

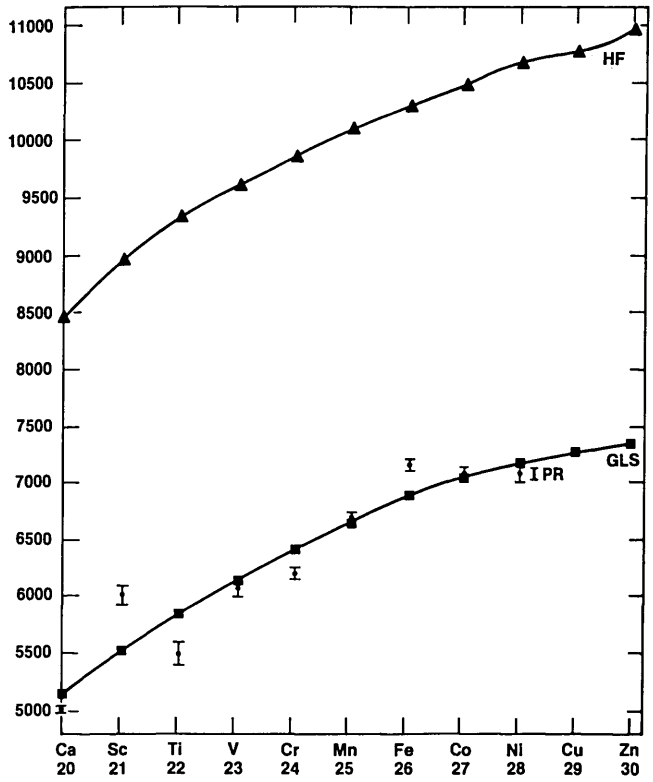

FIGURE 8. Plots of G_{ps} versus atomic number.

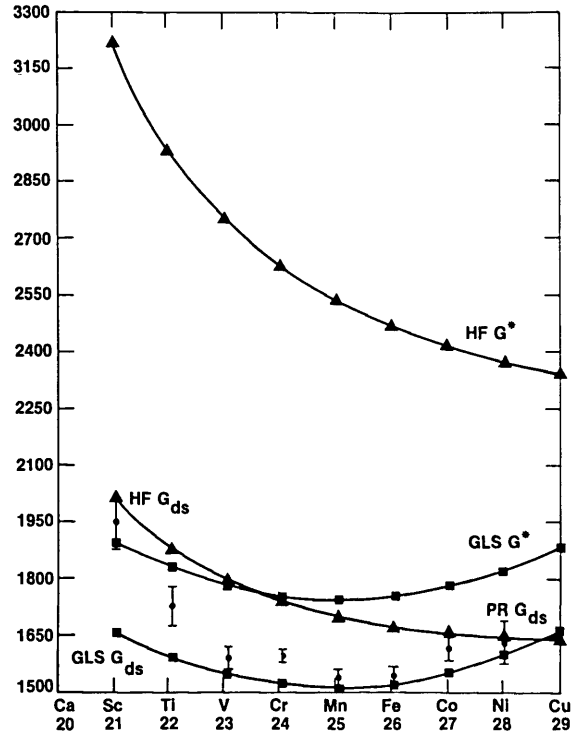

FIGURE 9. Plots of G_d, and G^* versus atomic number.

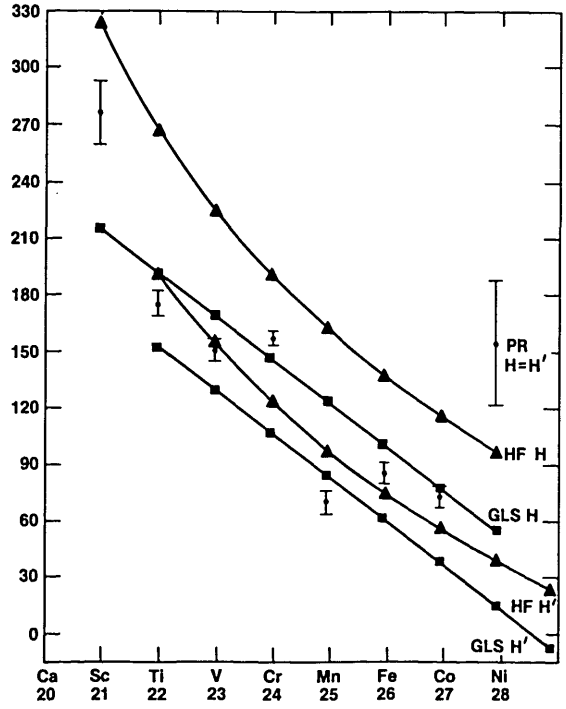

FIGURE 10. Plots of H and H' versus atomic number.

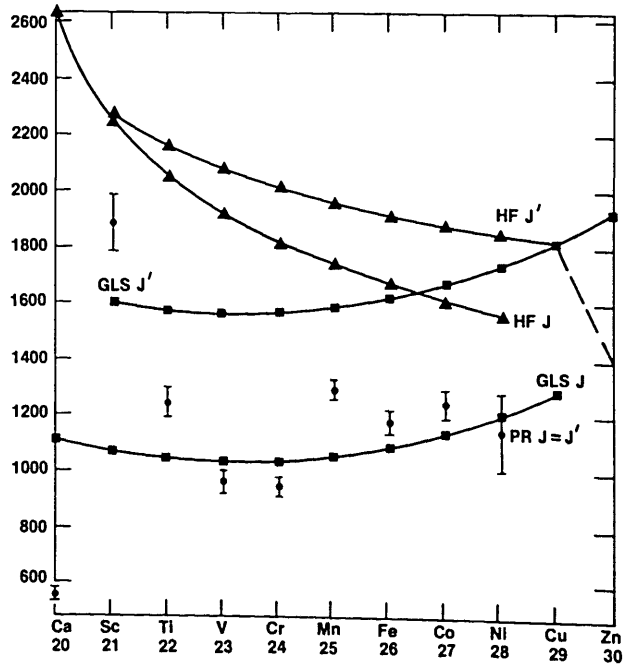

FIGURE 11. Plots of J and J' versus atomic number.

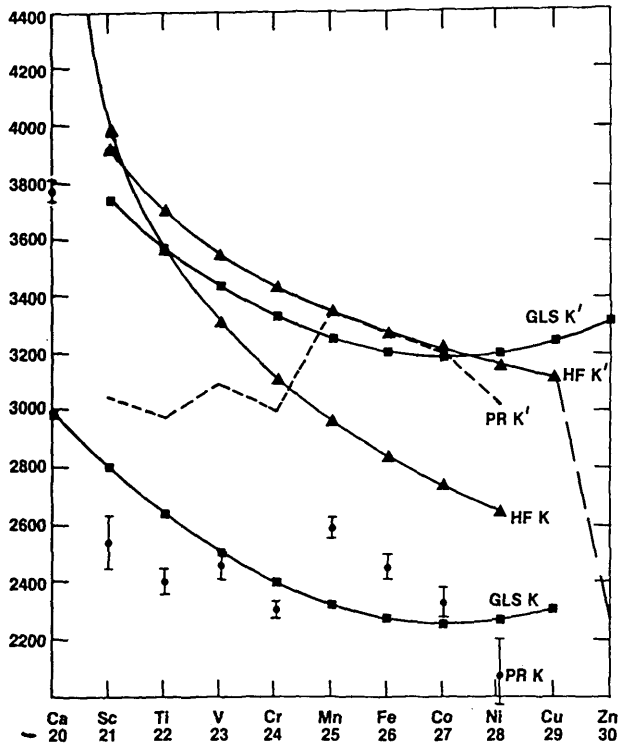

FIGURE 12. Plots of K and K' versus atomic number.

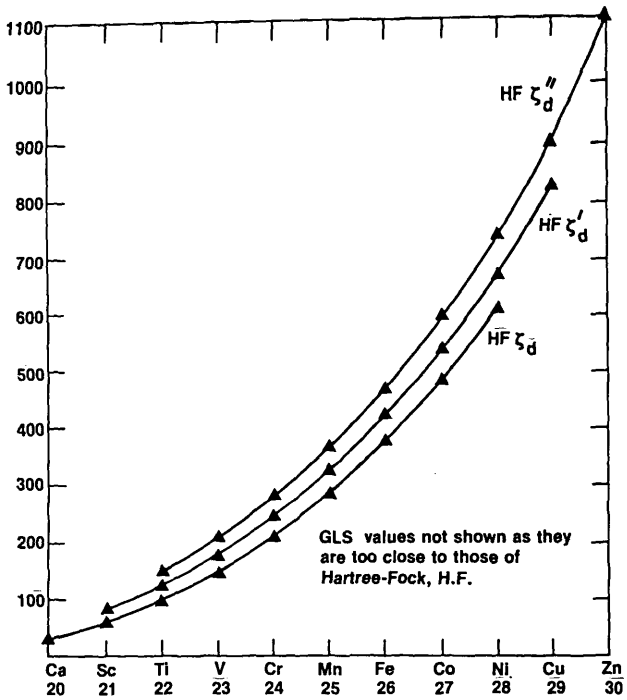

FIGURE 13. Plots of ζ_d, ζ_d', and ζ_d'' versus atomic number.

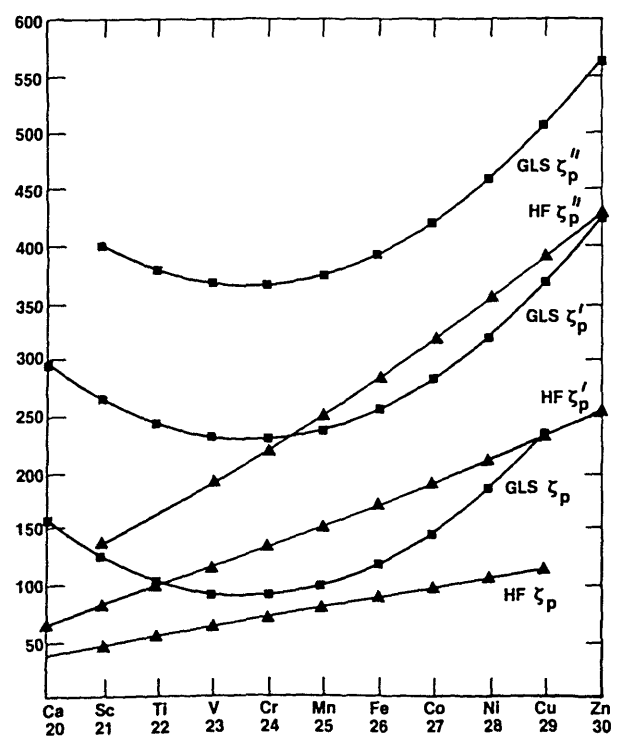

FIGURE 14. Plots of ζ_p, ζ_p', and ζ_p'' versus atomic number.

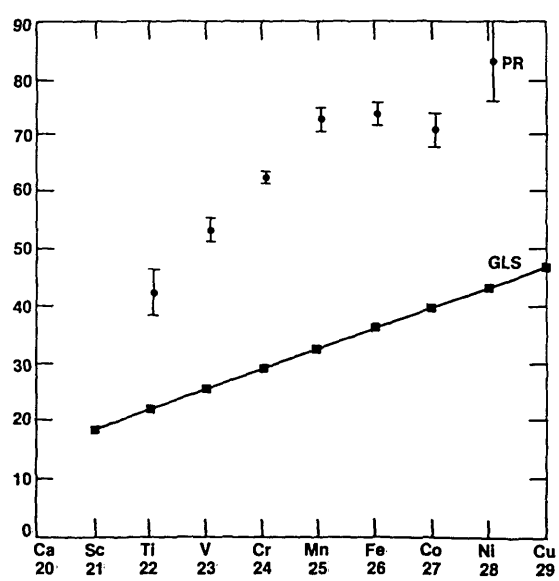

FIGURE 15. Plots of $\alpha = \alpha' = \alpha''$ versus atomic number.

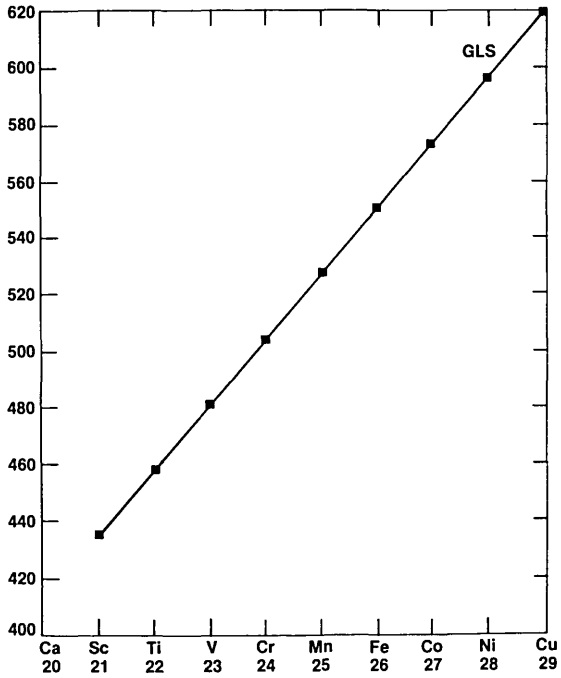

FIGURE 16. Plots of $\beta = \beta' = \beta''$ versus atomic number.

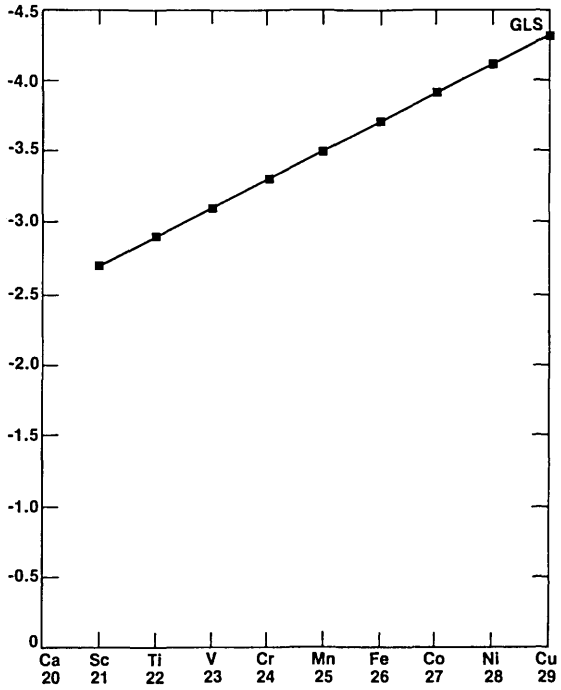

FIGURE 17. Plots of $T = T' = T''$ versus atomic number.